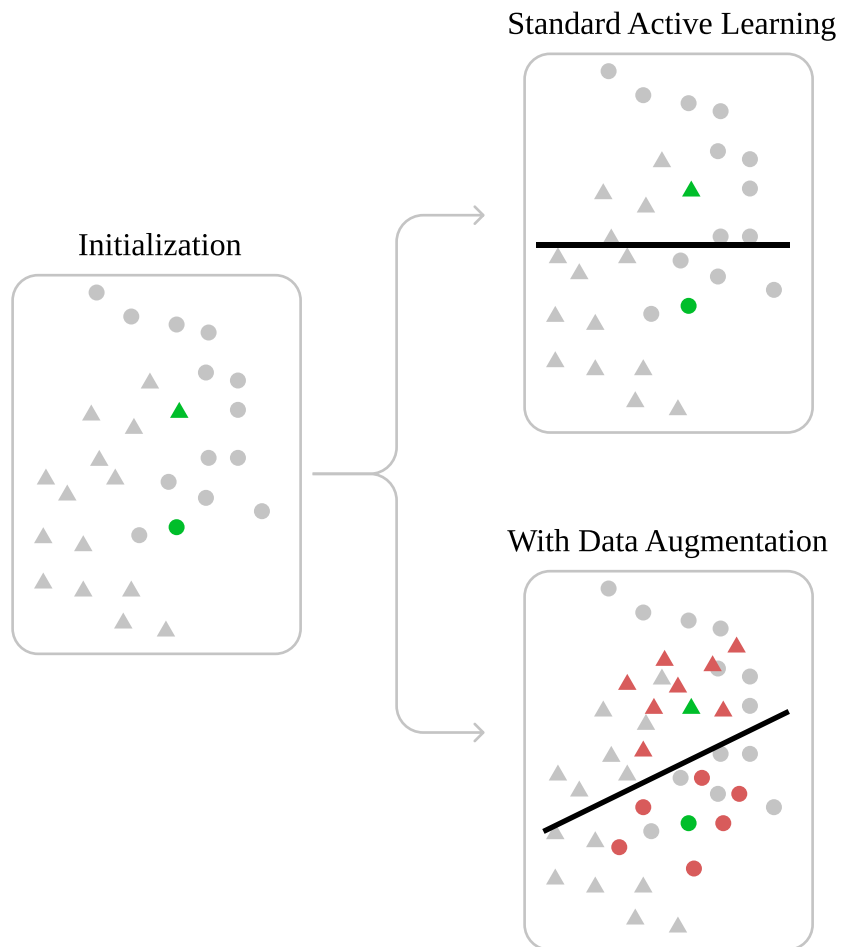


Graphical Abstract

Improving Active Learning Performance Through the Use of Data Augmentation

Joao Fonseca, Fernando Bacao



Highlights

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- We propose a new Active Learning framework that leverages hyperparameter optimization and data augmentation techniques;
- The use of data augmentation in Active Learning is sufficient to substantially improve the performance of an Active Learner, regardless of the choice of dataset/domain, classifier, or metric.
- In most scenarios, the proposed method outperformed classifiers trained in fully supervised settings while using less data.

Improving Active Learning Performance Through the Use of Data Augmentation

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Abstract

Active Learning (AL) is a technique that is used to iteratively select unlabeled observations out of a large pool of unlabeled data to be labeled by a supervisor. Its focus is to find the unlabeled observations that, once labeled, will maximize the informativeness of the training dataset. However, the manual labeling of observations involves human resources with domain expertise, making it an expensive and time-consuming task. The literature describes various methods to improve the effectiveness of this process, but there is little research developed around the usage of artificial data sources in AL. In this paper, we propose a new framework for AL, which allows the effective use of artificial data. Our method implements a data augmentation policy that optimizes the generation of artificial instances to improve the AL process. We compare the proposed method to the standard framework as well as another active learning method that uses data augmentation. The models' performance was tested using 4 different classifiers, 2 AL-specific performance metrics and 3 classification performance metrics over 10 different datasets. We show that the proposed framework, using data augmentation, significantly improves the performance of AL, both in terms of classification performance and data selection efficiency.

Keywords: Active Learning, Data Augmentation, Oversampling

1. Introduction

The importance of training robust ML models with minimal data requirements is substantially increasing [1, 2, 3]. Although the growing amount of

valuable data sources and formats being developed and explored is affecting various domains [4], this data is often unlabeled. Only a small amount of the data being produced and stored can be useful for supervised learning tasks. Additionally, it’s important to note that labeling data for specific Machine Learning (ML) projects is often difficult and expensive, especially when data-intensive ML techniques are involved (*e.g.*, Deep Learning classifiers) [1]. In this scenario, labeling the full dataset becomes impractical, time-consuming, and expensive. Two different ML techniques attempt to address this problem: Semi-Supervised Learning (SSL) and Active Learning (AL). Even though they address the same problem, the two follow different approaches. SSL focuses on observations with the most certain predictions, whereas AL focuses on observations with the least certain predictions [5].

SSL attempts to use a small, predefined set of labeled and unlabeled data to produce a classifier with superior performance. This method uses the unlabeled observations to help define the classifier’s decision boundaries [6]. Simultaneously, the amount of labeled data required to reach a given performance threshold is also reduced. It is a special case of ML because it falls between the supervised and unsupervised learning perspectives. AL, instead of optimizing the informativeness of an existing training set, it expands the dataset to include the most informative and/or representative observations [7]. It is an iterative process where a supervised model is trained and simultaneously identifies the most informative unlabeled observations to increase the performance of that classifier. The combination of SSL with AL has been explored in the past, achieving state-of-the-art results [8].

Several studies have pointed out the limitations of AL within an Imbalanced Learning context [9]. With imbalanced data, AL approaches frequently have low performance, high computational time, or data annotation costs. Studies addressing this issue tend to adopt classifier-level modifications, such as the Weighted Extreme Learning Machine [9, 10, 11]. However, classifier or query function-level modifications (See Section 2.1) have limited applicability since a universally good AL strategy has not been found [7]. Other methods address imbalance learning by weighing the observations as a function of the observation’s class imbalance ratio [12]. Alternatively, other methods reduce the imbalanced learning bias by combining Informative and Representative-based query approaches (see Section 2.1) [13]. Another approach to deal with imbalanced data and data scarcity, in general, is data augmentation. This approach has the advantage of being classifier-agnostic, potentially reduces the imbalanced learning bias, and also works as a reg-

ularization method in data-scarce environments, such as AL implementations [14]. However, most recent studies improve the AL performance by modifying the design/choice of the classifier and query functions used.

The usage of data augmentation in AL is not new. The literature found on the topic (see Section 2.3) focuses on either image classification or Natural Language Processing and uses Deep Learning-based data augmentation to improve the performance of neural network architectures in AL. These methods, although showing promising results, represent a limited perspective of the potential of data augmentation in a real-world setting. First, using Deep Learning in an iterative setting requires access to significant computational power. Second, these models tend to use sophisticated data augmentation methods, whose implementation may not be accessible to the non-sophisticated user. Third, the studies found on the topic are specific to the domain, classifier, and data augmentation method. Consequently, the direct effect of data augmentation is unclear: these studies implement different neural network-based techniques for different classification problems, whose performance may be attributed to various elements within the AL framework.

In this study, we explore the effect of data augmentation in AL in a context-agnostic setting, along with two different data augmentation policies: oversampling (where the amount of data generated for each class equals the amount of data belonging to the majority class) and non-constant data augmentation policies (where the amount of data generated exceeds the amount of data belonging to the majority class in varying quantities) between iterations. We start by conceptualizing the AL framework and each of its elements, as well as the modifications involved to implement data augmentation in the AL iterative process. We argue that simple, non-domain specific data augmentation heuristics are sufficient to improve the performance of AL implementations, without the need to resort to deep learning-based data augmentation algorithms.

When compared to the standard AL framework, the proposed framework contains two additional components: the Generator and the Hyperparameter Optimizer. We implement a modified version of Geometric Synthetic Minority Oversampling Technique (G-SMOTE) [15] as a data augmentation method with an optimized generation policy (explained in Section 2.2). We also propose a hyperparameter optimization module, which is used to find the best data augmentation policy at each iteration. We test the effectiveness of the proposed method in 10 datasets of different domains. We implement

3 AL frameworks (standard, oversampling and varying data augmentation) using 4 different classifiers, 3 different performance metrics and calculate 2 AL-specific performance metrics.

The rest of this manuscript is structured as follows: Section 2 introduces relevant topics discussed in the paper and describes the related work. Section 3 describes the proposed method. Section 4 describes the methodology of the study’s experiment. Section 5 presents the results obtained from the experiment, as well as a discussion of these results. Section 6 presents the conclusions drawn from this study.

2. Background

2.1. Active Learning

This paper focuses on pool-based AL methods as defined in [16]. The goal of AL models is to maximize the performance of a classifier, f_c , while annotating as least observations, x_i , as possible. They use a data pool, \mathcal{D} , where $\mathcal{D} = \mathcal{D}_{lab} \cup \mathcal{D}_{pool}$ and $|\mathcal{D}_{pool}| \gg |\mathcal{D}_{lab}|$. \mathcal{D}_{pool} and \mathcal{D}_{lab} refer to the sets of unlabeled and labeled data, respectively. Having a budget of T iterations (where $t = 1, 2, \dots, T$) and n annotations per iteration, at iteration t , f_c is trained using \mathcal{D}_{lab}^t to produce, for each $x_i \in \mathcal{D}_{pool}^t$, an uncertainty score using an acquisition function $f_{acq}(x_i; f_c)$. These uncertainty scores are used to annotate the n observations with highest ucertainity from \mathcal{D}_{pool}^t to form \mathcal{D}_{new}^t . The iteration ends with the update of $\mathcal{D}_{lab}^{t+1} = \mathcal{D}_{lab}^t \cup \mathcal{D}_{new}^t$ and $\mathcal{D}_{pool}^{t+1} = \mathcal{D}_{pool}^t \setminus \mathcal{D}_{new}^t$ [17, 2]. This process is shown in Figure 1. Before the start of the iterative process, assuming $\mathcal{D}_{lab}^{t=0} = \emptyset$, the data used to populate $\mathcal{D}_{lab}^{t=1}$ is typically collected randomly from $\mathcal{D} = \mathcal{D}_{pool}^{t=0}$ and is labeled by a supervisor [18, 19, 20].

Research focused on AL has typically been focused on the specification of f_{acq} and domain-specific applications. Acquisition functions can be divided into two different categories [21, 22]:

1. Informative-based. These strategies use the classifier’s output to assess the importance of each observation towards the performance of the classifier [23].
2. Representative-based. These strategies estimate the the optimal set of observations that will optimize the classifier’s performance [22].

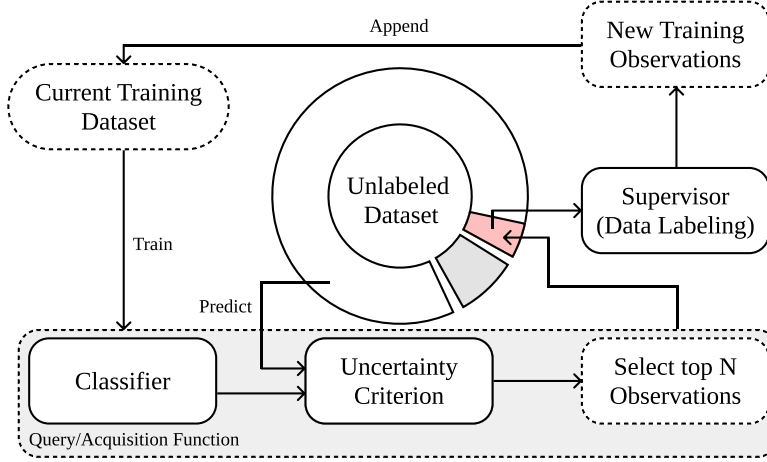


Figure 1: Diagram depicting a typical AL iteration. In the first iteration, the training set collected during the initialization process becomes the “Current Training Dataset”.

115 Although there are significant contributions toward the development of
 116 more robust query functions and classifiers in AL, modifications to AL’s
 117 basic structure are rarely explored. In [19] the authors introduce a loss
 118 prediction module in the AL framework to replace the uncertainty criterion.
 119 This model implements a second classifier to predict the expected loss of the
 120 unlabeled observations (using the actual losses collected during the training of
 121 the original classifier) and return the unlabeled observations with the highest
 122 expected loss. However, this contribution is specific to neural networks (and
 123 more specifically, to deep neural networks) and was only tested for image
 124 classification.

125 2.2. Data Augmentation

126
 127 Data Augmentation methods expand the training dataset by introducing
 128 new and informative observations [24]. The production of artificial data may
 129 be done via the introduction of perturbations on the input [25], feature [26],
 130 or output space [24]. Data Augmentation methods may be divided into two
 131 categories [27]:

- 132 1. Heuristic approaches attempt to generate new and relevant observa-
 133 tions through the application of a predefined procedure, usually incor-

porating some degree of randomness [28]. Since these methods typically occur in the input space, they require less data and computational power when compared to Neural Network methods.

2. Neural Network approaches, on the other hand, map the original input space into a lower-dimensional representation, known as the feature space [26]. The generation of artificial data occurs in the feature space and is reconstructed into the input space. Although these methods allow the generation of less noisy data in high-dimensional contexts and more plausible artificial data, they are significantly more computationally intensive.

While some techniques may depend on the domain, others are domain-agnostic. For example, Random Erasing [25], Translation, Cropping and Flipping are examples of image data-specific augmentation methods. Other methods, such as autoencoders, may be considered domain agnostic.

2.3. Data Augmentation in Active Learning

The standard AL model can be complemented with a data augmentation function, $f_{aug}(x_i; \tau)$, where τ defines the augmentation policy. In this context, τ refers to the transformation applied and its hyperparameters and $f_{aug}(x; \tau) : \mathcal{D} \rightarrow \mathcal{D}_{aug}(\mathcal{D})$ produces a modified observation, $\tilde{x} \in \mathcal{D}_{aug}(\mathcal{D})$ where $\mathcal{D}_{aug}(\mathcal{D})$ is the set of modified observations. This involves the usage of a new set of data, $\mathcal{D}_{train}^t = \mathcal{D}_{lab}^t \cup \mathcal{D}_{aug}^t$, to train the classifier.

As found in Section 2.1, improvements proposed in the AL framework are mostly focused on modifications of the classifier or query strategy. Furthermore, the few recent AL contributions implementing data augmentation were all (except one) applied to the computer vision or natural language processing (NLP) realm.

The only AL model found that uses data augmentation outside of the computer vision or NLP domains uses a pipelined approach, described in [18]. In this study, the AL model proposed is applied for tabular data using an oversampling data augmentation policy (*i.e.*, the artificial data was generated only to balance the target class frequencies). However, this AL model was applied in a Land Use/Land Cover context with specific characteristics that are not necessarily found in other supervised learning problems. Specifically, these types of datasets are high dimensional and have limited data variability

within each class (*i.e.*, cohesive spectral signatures within classes) due to their geographical proximity. Furthermore, this method does not allow augmentation policy optimization (*i.e.*, every hyperparameter has to be hardcoded a priori).

The Bayesian Generative Active Deep Learning (BGDAL) [29] is another example of a pipelined combination of f_{acq} and f_{aug} , applied image classification. BGDAL uses a Variational AutoEncoder (VAE) architecture to generate artificial observations. However, the proposed model is computationally expensive, requires a large data pool to train the VAE, and is not only dependent on the quality of the augmentations performed, but also on the performance of the discriminator and classifiers used.

The method proposed in [14], Look-Ahead Data Acquisition for Deep Active Learning, implement data augmentation to train a deep-learning classifier. However, adapting existing AL applications to use this approach is often impractical and implies the usage of image data, since the augmentations used are image data specific and occur on the unlabeled observations, before the unlabeled data selection.

The Variational Adversarial Active Learning (VAAL) model [30] is a deep AL approach to image classification that uses as inputs the embeddings produced by a VAE into a secondary classifier, working as f_{acq} , to predict if $x_i \in \mathcal{D}$ belongs to \mathcal{D}_{pool} . The n true positives with the highest certainty are labeled by the supervisor and \mathcal{D}_{pool} and \mathcal{D}_{lab} are updated as described in Section 2.1. The Task-aware VAAL model [31] extends the VAAL model by introducing a ranker, which consists of the Learning Loss module introduced in [19]. These models use data augmentation techniques to train the different neural network-based components of the proposed models. However, the AL components used are specific image classification, computationally expensive and the analysis of the effect of data augmentation in these AL models is not discussed.

In [32] the proposed AL method was designed specifically for image data classification, where a deep learning model was implemented as a classifier, but its architecture is not described, the augmentation policies used are unknown and the results reported correspond to single runs of the discussed model. The remaining AL models found implementing data augmentation were introduced for NLP applications, in [33, 34]. However, these methods were designed for specific applications within that domain and are not necessarily transferable to other domains or tasks.

206 3. Proposed Method

207

208 Based on the literature found on AL, most of the contributions and
209 novel implementations of AL algorithms focused on the improvement of the
210 choice/architecture of the classifier or the improvement of the uncertainty
211 criterion. In addition, the resulting classification performance of AL-trained
212 classifiers is frequently inconsistent and marginally improve the classifica-
213 tion performance when compared to classifiers trained over the full training
214 set. In addition, there is also a significant variability of the data selection
215 efficiency during different runs of the AL iterative process [18].

216 This paper provides a context-agnostic AL framework for the integration
217 of Data Augmentation within AL, with the following contributions:

- 218 1. Improvement of the AL framework by introducing a parameter tuning
219 stage using only the labeled dataset available at the current iteration
220 (*i.e.*, no labeled hold-out set is needed).
- 221 2. Generalization of the generator module proposed in [18] from oversam-
222 pling techniques to any other data augmentation mechanism and/or
223 policy.
- 224 3. Implementation of data augmentation outside of the Deep AL realm,
225 which was not previously found in the literature.
- 226 4. Analysis of the impact of Data Augmentation and Oversampling in AL
227 over 10 different datasets of different domains, while comparing them
228 with the standard AL framework.

229 The proposed AL framework is depicted in Figure 2. The generator el-
230 ement becomes an additional source of data and is expected to introduce
231 additional data variability into the training dataset. This should allow the
232 classifier to generalize better and perform more consistently over unseen ob-
233 servations. However, in this scenario, the amount of data to generate per
234 class at each iteration is unknown. Consequently, the hyperparameter tun-
235 ing step was introduced to estimate the optimal data augmentation policy
236 at each iteration. In our implementation, this step uses the current training
237 dataset to perform an exhaustive search over specified parameters of the gen-
238 erator, tested over a 5-fold cross-validation method. The best augmentation

239 policy found is used to train the iteration’s classifier in the following step.
 240 This procedure is described in Algorithm 1.

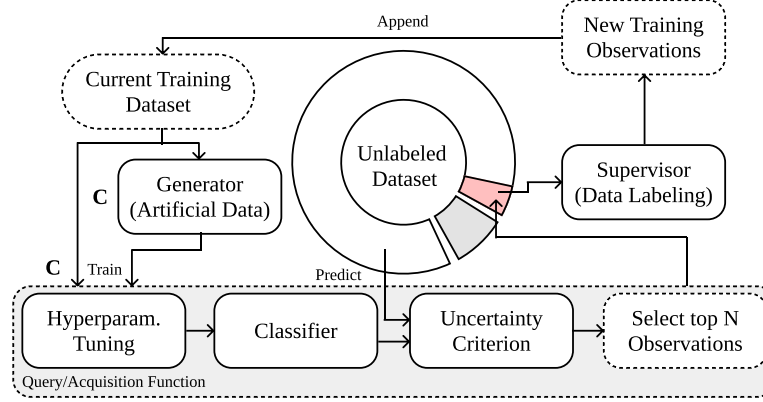


Figure 2: Diagram depicting the proposed AL iteration. The proposed modifications are marked with a boldface “C”.

241 To show the effectiveness of data augmentation in an AL implementation,
 242 we implemented a simple modification in the selection mechanism of the G-
 243 SMOTE algorithm. We use the uncertainties produced by f_{acq} to compute
 244 the probabilities of observations to be selected for augmentation, as an ad-
 245 ditional parameter. This modification is described in Algorithm 2

246 This modification facilitates the usage of G-SMOTE beyond its origi-
 247 nal oversampling purposes. However, in this paper, the data augmentation
 248 strategies are also used to ensure that class frequencies are balanced. Fur-
 249 thermore, the amount of artificial data produced for each class is defined
 250 by the *augmentation factor*, α_{af} , which represents a percentage of the ma-
 251 jority class C_{maj} (e.g., an augmentation factor of 1.2 will ensure there are
 252 $\text{count}(C_{maj}) \times 1.2$ observations in every class). In this paper’s experiment,
 253 the data generation mechanism is similar to the one in [18]. This allows the
 254 direct comparison of the two frameworks and establishes a causality of the
 255 performance variations to the data generation mechanism (i.e., augmentation
 256 vs normal oversampling) and hyperparameter tuning steps. However, in this
 257 case, the hyperparameter tuning is only going to be used for augmentation
 258 policy optimization.

Algorithm 1: Proposed AL Framework (Single iteration)

Given: $t \geq 1$, performance metric f_{pm}
Input: $\mathcal{D}_{pool}, \mathcal{D}_{lab}, f_c, f_{aug}, f_{acq}, \tau_{grid}, k, n$
Output: $\mathcal{D}_{pool}, \mathcal{D}_{lab}$

```

1 Function ParameterTuning( $f_c, f_{aug}, \tau_{grid}, \mathcal{D}_{lab}, k$ ):
2    $p \leftarrow 0$ 
3    $\tau \leftarrow \emptyset$ 
4    $\{\mathcal{D}_{lab}^1, \dots, \mathcal{D}_{lab}^k\} \leftarrow \mathcal{D}_{lab}$       //  $\mathcal{D}_{lab}^n \cap \mathcal{D}_{lab}^m = \emptyset, \forall (n, m) \in 1, \dots, k$ 
5   forall  $\tau' \in \tau_{grid}$  do
6      $p' \leftarrow \emptyset$ 
7     forall  $\mathcal{D}_{lab}^i \in \{\mathcal{D}_{lab}^1, \dots, \mathcal{D}_{lab}^k\}$  do
8        $\mathcal{D}'_{test} \leftarrow \mathcal{D}_{lab}^i$ 
9        $\mathcal{D}'_{train} \leftarrow \mathcal{D}_{lab} \setminus \mathcal{D}_{lab}^i$ 
10       $\mathcal{D}'_{train} \leftarrow f_{aug}(\mathcal{D}'_{train}; \tau')$ 
11      train  $f_c$  using  $\mathcal{D}'_{train}$ 
12       $p' \leftarrow p' \cup \{f_{pm}(f_c(\mathcal{D}_{test}))\}$ 
13     $p' \leftarrow \frac{\sum_{x_i \in p'} x_i}{k}$ 
14    if  $p' > p$  then
15       $p \leftarrow p'$ 
16       $\tau \leftarrow \tau'$ 
17  return  $\tau$ 
18 begin
19    $\tau \leftarrow \text{ParameterTuning}(f_c, f_{aug}, \tau_{grid}, \mathcal{D}_{lab}, k)$ 
20    $\mathcal{D}_{train} \leftarrow f_{aug}(\mathcal{D}_{lab}; \tau)$ 
21   train  $f_c$  using  $\mathcal{D}_{train}$ 
22    $\mathcal{D}_{new} = \arg \max_{\mathcal{D}'_{pool} \subset \mathcal{D}_{pool}, |\mathcal{D}'_{pool}|=n} \sum_{x \in \mathcal{D}'_{pool}} f_{acq}(x; f_c)$ 
23   annotate  $\mathcal{D}_{new}$ 
24    $\mathcal{D}_{pool} \leftarrow \mathcal{D}_{pool} \setminus \mathcal{D}_{new}$ 
25    $\mathcal{D}_{lab} \leftarrow \mathcal{D}_{lab} \cup \mathcal{D}_{new}$ 

```

Algorithm 2: G-SMOTE Modified for Data Augmentation in AL

Given: $t \geq 1$, $\mathcal{D}_{lab}^t \neq \emptyset$, $\mathcal{D}_{lab} = \mathcal{D}_{lab}^{min} \cup \mathcal{D}_{lab}^{maj}$, $GSMOTE$
Input: \mathcal{D}_{pool}^t , \mathcal{D}_{lab}^t , f_c^{t-1} , f_{acq} , τ
Output: \mathcal{D}_{train}^t

```

1 Function  $DataSelection(\mathcal{D}_{lab}^t, f_{acq}, f_c^{t-1})$ :
2    $U \leftarrow \emptyset$ 
3    $P \leftarrow \emptyset$ 
4    $p_s \sim \mathcal{U}(0, 1)$ 
5   forall  $x_i \in \mathcal{D}_{lab}^t$  do
6      $u_{x_i} \leftarrow f_{acq}(x_i; f_c^{t-1})$ 
7      $U \leftarrow U \cup \{u_{x_i}\}$ 
8   forall  $u_{x_i} \in U$  do
9      $p_{x_i} \leftarrow \frac{u_{x_i}}{\sum U} + \sum P$ 
10     $P \leftarrow P \cup \{p_{x_i}\}$ 
11     $i \leftarrow \operatorname{argmax}(P < p_s)$ 
12    return  $i$ -th element in  $\mathcal{D}_{lab}^t$ 
13 begin
14    $\mathcal{D}_{aug}^{min} \leftarrow \emptyset$ 
15    $\mathcal{D}_{aug}^{maj} \leftarrow \emptyset$ 
16    $\alpha_{af}, \alpha_{trunc}, \alpha_{def} \leftarrow \tau$ 
17    $N \leftarrow \operatorname{count}(C_{maj}) \times \alpha_{af}$ 
18   forall  $\mathcal{D}'_{aug} \in \{\mathcal{D}_{aug}^{min}, \mathcal{D}_{aug}^{maj}\}$ ,  $\mathcal{D}'_{lab} \in \{\mathcal{D}_{lab}^{min}, \mathcal{D}_{lab}^{maj}\}$  do
19     while  $|\mathcal{D}'_{aug}| < N$  do
20        $x_{center} \leftarrow DataSelection(\mathcal{D}'_{lab}, f_{acq}, f_c^{t-1})$ 
21        $x_{gen} \leftarrow GSMOTE(x_{center}, \mathcal{D}'_{lab}, \alpha_{trunc}, \alpha_{def})$ 
22        $\mathcal{D}'_{aug} \leftarrow \mathcal{D}'_{aug} \cup \{x_{gen}\}$ 
23    $\mathcal{D}_{aug} \leftarrow \mathcal{D}_{aug}^{min} \cup \mathcal{D}_{aug}^{maj}$ 
24    $\mathcal{D}_{train}^t \leftarrow \mathcal{D}_{lab}^t \cup \mathcal{D}_{aug}$ 

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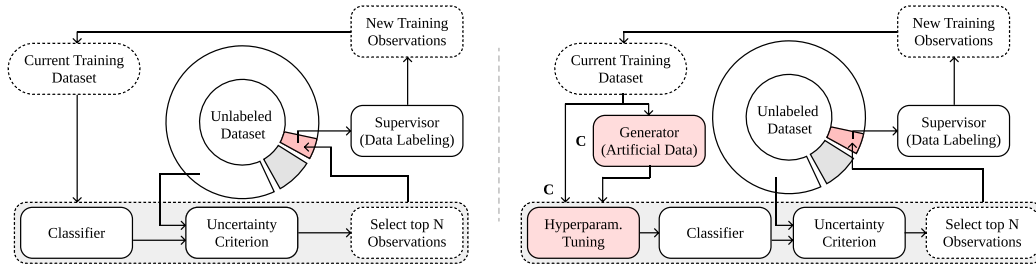


Figure 3: Simplified diagrams highlighting the differences between the proposed and standard AL iterations. The proposed modifications are **highlighted** in red and marked with a boldface “C”.

259 The comparison of diagrams between the proposed and standard AL
 260 frameworks is shown in Figure 3. In the proposed framework, we (1) gen-
 261 eralize the generator module to accept any data augmentation method or
 262 policy and (2) a hyperparameter tuning module to estimate the optimal
 263 data augmentation policy. This framework was designed to be task-agnostic.
 264 Specifically, any data augmentation method (domain-specific or not) may be
 265 used, as well as any other parameter search method. It is also expected to
 266 be compatible with other AL modifications, including the ones that do not
 267 affect solely the classifier or uncertainty criterion, such as the one proposed
 268 in [19].

269 4. Methodology

270
 271 This section describes the different elements included in the experimen-
 272 tal procedure. The datasets used were acquired in open data repositories.
 273 **Their** sources and preprocessing steps are defined in Subsection 4.1. The
 274 classifiers used in the experiment are defined in Subsection 4.2. The metrics
 275 chosen to measure AL performance and overall classification performance are
 276 defined in Subsection 4.3. The experimental procedure is described in Sub-
 277 section 4.4. The implementation of the experiment and resources used to do
 278 so are described in Subsection 4.5.

279 The methodology developed serves 2 purposes: (1) Compare classification
 280 performance once all the AL procedures are completed (*i.e.*, optimal perfor-
 281 mance of a classifier trained via iterative data selection) and (2) Compare
 282 the amount of data required to reach specific performance thresholds (*i.e.*,

the number of AL iterations required to reach similar classification performances).

4.1. Datasets

The datasets used to test the proposed method are publicly available in open data repositories. Specifically, they were retrieved from OpenML and the UCI Machine Learning Repository. They were chosen considering different domains of application, imbalance ratios, dimensionality and number of target classes, all of them focused on classification tasks. The goal is to demonstrate the performance of the different AL frameworks in various scenarios and domains. The data preprocessing approach was similar across all datasets. Table 1 describes the key properties of the 10 preprocessed datasets where the experimental procedure was applied.

Dataset	Features	Instances	Minority instances	Majority instances	IR	Classes
Image Segmentation	14	1155	165	165	1.0	7
Mfeat Zernike	47	1994	198	200	1.01	10
Texture	40	1824	165	166	1.01	11
Waveform	40	1666	551	564	1.02	3
Pendigits	16	1832	176	191	1.09	10
Vehicle	18	846	199	218	1.1	4
Mice Protein	69	1073	105	150	1.43	8
Gas Drift	128	1987	234	430	1.84	6
Japanese Vowels	12	1992	156	323	2.07	9
Baseball	15	1320	57	1196	20.98	3

Table 1: Description of the datasets collected after data preprocessing. The sampling strategy is similar across datasets. Legend: (IR) Imbalance Ratio

The data preprocessing pipeline is depicted as a flowchart in Figure 4. The missing values are removed from each dataset by removing the corresponding observations. This ensures that the input data in the experiment is kept as close to its original form as possible. The non-metric features (*i.e.*, binary, categorical, and ordinal variables) were removed since the application of G-SMOTE is limited to continuous and discrete features. The datasets containing over 2000 observations were downsampled in order to maintain the datasets to a manageable size. The data sampling procedure preserves

304 the relative class frequency of the dataset, in order to maintain the Imbal-
 305 ance Ratio (IR) originally found in each dataset (where $IR = \frac{\text{count}(C_{maj})}{\text{count}(C_{min})}$).
 306 The remaining features of each dataset are scaled to the range of $[-1, 1]$ to
 307 ensure a common range across features.

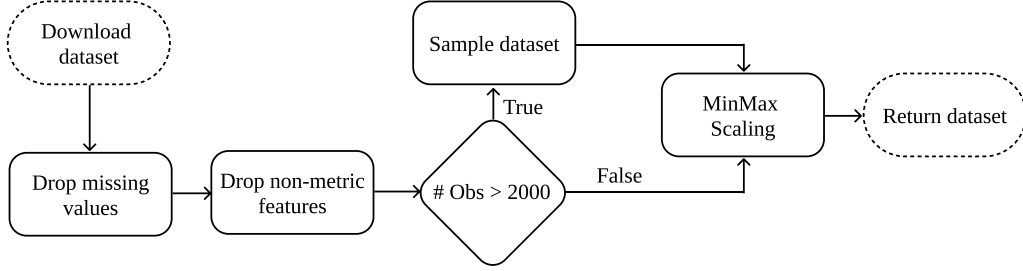


Figure 4: Data preprocessing pipeline.

308 The preprocessed datasets were stored into a SQLite database file and is
 309 available along with the experiment’s source code in the GitHub repository
 310 of the project (see Subsection 4.5).

311 4.2. Machine Learning Algorithms

312
 313 We used a total of 4 classification algorithms and a heuristic data aug-
 314 mentation mechanism. The choice of classifiers was based on the popularity
 315 and family of the classifiers (tree-based, nearest neighbors-based, ensemble-
 316 based and linear models). Our proposed method was tested using a Decision
 317 Tree (DT) [35], a K-nearest neighbors classifier (KNN) [36], a Random For-
 318 est Classifier (RF) [37] and a Logistic Regression (LR) [38]. Since the target
 319 variables are multi-class, the LR classifier was implemented using the one-
 320 versus-all approach. The predicted class is assigned to the label with the
 321 highest likelihood.

322 The oversampler G-SMOTE was used as a data augmentation method.
 323 The typical data generation policy of oversampling methods is to generate
 324 artificial observations on non-majority classes such that the number of major-
 325 ity class observations matches those of each non-majority class. We modified
 326 this data generation policy to generate observations for all classes, as a per-
 327 centage of the number of observations in the majority class. In addition, the

original G-SMOTE algorithm was modified to accept data selection probabilities based on classification uncertainty. These modifications are discussed in Section 3.

Every AL procedure was tested with different selection criteria: Random Selection, Entropy, and Breaking Ties. The baseline used is the standard AL procedure. As a benchmark, we add the AL procedure using G-SMOTE as a normal oversampling method, as proposed in [18]. Our proposed method was implemented using G-SMOTE as a data augmentation method to generate artificial observations for all classes, while still balancing the class distribution, as described in Section 3.

4.3. Evaluation Metrics

Considering the imbalanced nature of the datasets used in the experiment, commonly used performance metrics such as Overall Accuracy (OA), although being intuitive to interpret, are insufficient to quantify a model’s classification performance [39]. The Cohen’s Kappa performance metric, similar to OA, is also biased towards high-frequency classes since its definition is closely related to the OA metric, making its behavior consistent with OA [40]. However, these metrics remain popular choices for the evaluation of classification performance. Other performance metrics like $Precision = \frac{TP}{TP+TN}$, $Recall = \frac{TP}{TP+FN}$ or $Specificity = \frac{TN}{TN+FP}$ are calculated as a function of True/False Positives (TP and FP) and True/False Negatives (TN and FN) and can be used at a per-class basis instead. In a multiple dataset scenario with varying amount of target classes and meanings, comparing the performance of different models using these metrics becomes impractical.

Based on the recommendations found in [39, 41], we used 2 metrics found to be less sensitive to the class imbalance bias, along with OA as a reference for easier interpretability:

- The Geometric-mean scorer (G-mean) consists of the geometric mean of Specificity and Recall [41]. Both metrics are calculated in a multiclass context considering a one-versus-all approach. For multiclass problems, the G-mean scorer is calculated as its average per class values:

$$G\text{-mean} = \sqrt{\overline{Sensitivity} \times \overline{Specificity}}$$

- The F-score metric consists of the harmonic mean of Precision and Recall. The two metrics are also calculated considering a one-versus-all approach. The F-score for the multi-class case can be calculated using its average per class values [39]:

$$F\text{-score} = 2 \times \frac{\overline{Precision} \times \overline{Recall}}{\overline{Precision} + \overline{Recall}}$$

- The OA consists of the number of TP divided by the total amount of observations. Considering c as the label for the different classes present in a target class, OA is given by the following formula:

$$OA = \frac{\sum_c TP_c}{\sum_c (TP_c + FP_c)}$$

The comparison of the performance of AL frameworks is based on its data selection and augmentation efficacy. Specifically, an efficient data selection/generation policy allows the production of classifiers with high performance on unseen data while using as least non-artificial training data as possible. To measure the performance of the different AL setups, we follow the recommendations found in [42]. The performance of an AL setup will be compared using two AL-specific performance metrics:

- Area Under the Learning Curve (AULC). It is the sum of the classification performance over a validation/test set of the classifiers trained of all AL iterations. To facilitate the interpretability of this metric, the resulting AULC scores are fixed within the range $[0, 1]$ by dividing the AULC scores by the total amount of iterations (*i.e.*, the maximum performance area).
- Data Utilization Rate (DUR) [43]. Measures the percentage of training data required to reach a given performance threshold, as a ratio of the percentage of training data required by the baseline framework. This metric is also presented as a percentage of the total amount of training data, without making it relative to the baseline framework. The DUR metric is measured at 45 different performance thresholds, ranging between $[0.10, 1.00]$ at a 0.02 step.

387 4.4. Experimental Procedure

388

389 The evaluation of different active learners in a live setting is generally
390 expensive, time-consuming, and prone to human error. Instead, a com-
391 mon practice is to compare them in an offline environment using labeled
392 datasets [44]. In this scenario, since the dataset is already labeled, the anno-
393 tation process is done at zero cost. Figure 5 depicts the experiment designed
394 for one dataset over a single run.

395 A single run starts with the splitting of a preprocessed dataset in 5 dif-
396 ferent partitions, stratified according to the class frequencies of the target
397 variable using the K-fold Cross Validation method. During this run, an ac-
398 tive learner or classifier is trained 5 times using a different partition as the
399 Test set each time. For each training process, a Validation set containing 25%
400 of the subset is created and is used to measure the data selection efficiency
401 (*i.e.*, AULC and DUR using the classification performance metrics, specific
402 to AL). Therefore, for a single training procedure, 20% of the original dataset
403 is used as the Validation set, 20% is used as the Test set and 60% is used as
404 the Train set. The AL simulations and the classifiers' training occur within
405 the Train set. However, the classifiers used to find the maximum performance
406 classification scores are trained over the full Train set. The AL simulations
407 are run over a maximum of 50 iterations (including the initialization step),
408 adding 1.6% of the training set each time (*i.e.*, all AL simulations use less
409 than 80% of the Train set). Once the training phase is completed, the Test
410 set classification scores are calculated using the trained classifiers. For the
411 case of AL, the classifier with the optimal Validation set score is used to
412 estimate the AL's optimal classification performance over unseen data.

413 The process shown in Figure 5 is repeated over 3 runs using different
414 random seeds over the 10 different datasets collected. The final scores of
415 each AL configuration and classifier correspond to the average of the 3 runs
416 and 5-fold Cross-Validation estimations (*i.e.*, the mean score of 15 fits, across
417 10 datasets).

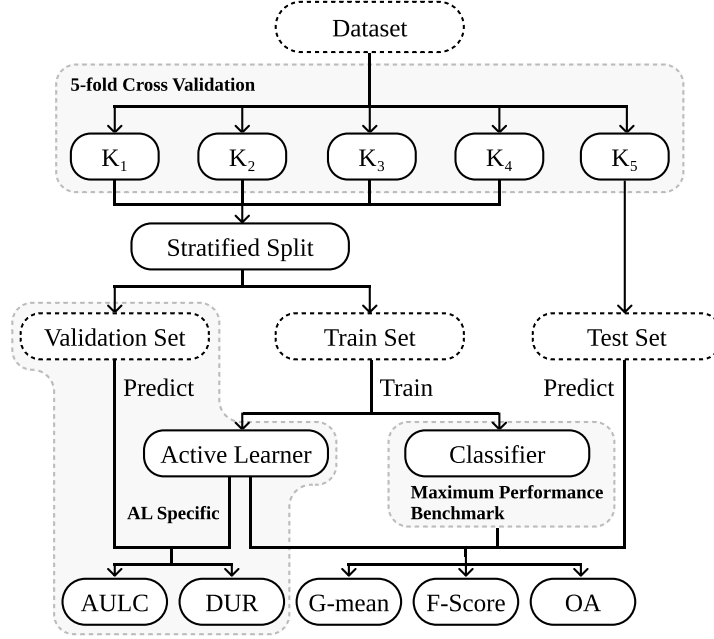


Figure 5: Experimental procedure flowchart. The preprocessed datasets are split into five folds. One of the folds is used to test the best-found classifiers using AL and the classifiers trained using the entire training dataset (containing the remaining folds). The training set is used to run both the AL simulations as well as train the normal classifiers. The validation set is used to measure AL-specific performance metrics over each iteration. We use different subsets for overall classification performance and AL-specific performance to avoid data leakage.

418 The hyperparameters defined for the AL frameworks, Classifiers, and
419 Generators are shown in Table 2. In the Generators table, we distinguish
420 the G-SMOTE algorithm working as a normal oversampling method from G-
421 SMOTE-AUGM, which performs generates additional artificial data on top
422 of the usual oversampling mechanism. Since the G-SMOTE-AUGM method
423 is intended to be used with varying parameter values (via within-iteration
424 parameter tuning), the parameters were defined as a list of various possible
425 values.

Active Learners	Hyperparameters	Inputs
Standard	# initial obs.	1.6%
	# additional obs. per iteration	1.6%
	max. iterations + initialization	50
	evaluation metrics	G-mean, F-score, OA
	selection strategy	Random, Entropy, Breaking Ties
	within-iteration param. tuning	None
	generator	None
	classifier	DT, LR, KNN, RF
Oversampling	generator	G-SMOTE
Proposed	generator	G-SMOTE-AUGM
	within-iteration param. tuning	Grid Search K-fold CV
Classifier		
DT	min. samples split	2
	criterion	gini
LR	maximum iterations	100
	multi class	One-vs-All
	solver	liblinear
KNN	penalty	L2 (Ridge)
	# neighbors	5
	weights	uniform
RF	metric	euclidean
	min. samples split	2
	# estimators	100
	criterion	gini
Generator		
G-SMOTE	# neighbors	4
	deformation factor	0.5
	truncation factor	0.5
G-SMOTE-AUGM	# neighbors	3, 4, 5
	deformation factor	0.5
	truncation factor	0.5
	augmentation factor	[1.1, 2.0] at 0.1 step

Table 2: Hyperparameter definition for the active learners, classifiers, and generators used in the experiment.

426 4.5. Software Implementation

427

428 The experiment was implemented using the Python programming lan-
429 guage, along with the Python libraries Scikit-Learn [45], Imbalanced-Learn [46],
430 Geometric-SMOTE [15], Research-Learn and ML-Research libraries. All
431 functions, algorithms, experiments, and results are provided in the GitHub
432 repository of the project.

433 5. Results & Discussion

434

435 In a multiple dataset experiment, the analysis of results should not rely
436 uniquely on the average performance scores across datasets. The domain of
437 application and fluctuations of performance scores between datasets make the
438 analysis of these averaged results less accurate. Instead, it is generally rec-
439 ommended to use the mean ranking scores to extend the analysis [47]. Since
440 mean performance scores are still intuitive to interpret, we will present and
441 discuss both results. The rank values are assigned based on the mean scores
442 of 3 different runs of 5-fold Cross-Validation (15 performance estimations
443 per dataset) for each combination of dataset, AL configuration, classifier,
444 and performance metric.

445 5.1. Results

446

447 The average rankings of the AULC estimations of AL methods are shown
448 in Table 3. The proposed method almost always improves AL performance
449 and ensures higher data selection efficiency.

Classifier	Evaluation Metric	Standard	Oversampling	Proposed
DT	Accuracy	2.50 ± 0.81	2.20 ± 0.40	1.30 ± 0.64
DT	F-score	2.50 ± 0.81	2.10 ± 0.30	1.40 ± 0.80
DT	G-mean	2.70 ± 0.64	2.00 ± 0.45	1.30 ± 0.64
KNN	Accuracy	2.40 ± 0.80	1.90 ± 0.54	1.70 ± 0.90
KNN	F-score	2.60 ± 0.66	1.80 ± 0.40	1.60 ± 0.92
KNN	G-mean	2.80 ± 0.40	1.70 ± 0.46	1.50 ± 0.81
LR	Accuracy	2.60 ± 0.66	2.10 ± 0.54	1.30 ± 0.64
LR	F-score	2.80 ± 0.40	2.00 ± 0.45	1.20 ± 0.60
LR	G-mean	2.80 ± 0.40	2.00 ± 0.45	1.20 ± 0.60
RF	Accuracy	2.60 ± 0.66	1.90 ± 0.54	1.50 ± 0.81
RF	F-score	2.60 ± 0.66	2.00 ± 0.45	1.40 ± 0.80
RF	G-mean	2.80 ± 0.40	1.60 ± 0.49	1.60 ± 0.80

Table 3: Mean rankings of the AULC metric over the different datasets (10), folds (5) and runs (3) used in the experiment. The proposed method always improves the results of the original framework and on average almost always improves the results of the oversampling framework.

Table 4 shows the average AULC scores, grouped by classifier, Evaluation Metric, and AL framework. The variation in performance across active learners is consistent with the mean rankings found in Table 3, while showing significant AULC score differences between the proposed AL method and the oversampling AL method.

The average DUR scores were calculated for various G-mean thresholds, varying between 0.1 and 1.0 at a 0.02 step (45 different thresholds in total). Table 5 shows the results obtained for these scores starting from a G-mean score of 0.6 and was filtered to show only the thresholds ending with 0 or 6. In most cases, the proposed method reduces the amount of data annotation required to reach each G-mean score threshold.

The DUR scores relative to the Standard AL method are shown in Figure 6. A DUR below 1 means that the Proposed/Oversampling method requires less data than the Standard AL method to reach the same performance threshold. For example, running an AL simulation using the KNN classifier requires 69.6% of the amount of data required by the Standard AL method using the same classifier to reach an F-Score of 0.62 (*i.e.*, requires 30.4% less data).

The mean optimal classification scores of AL methods and Classifiers

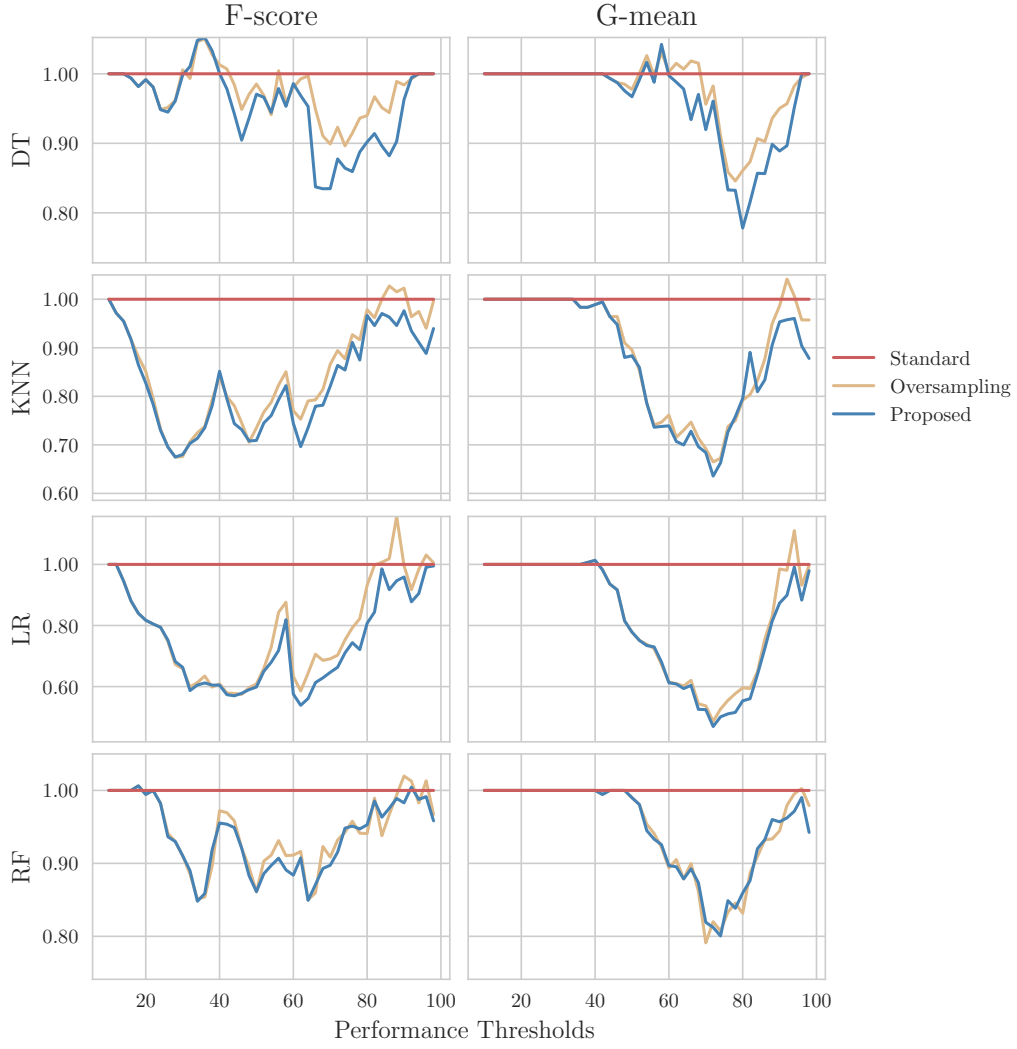


Figure 6: Mean data utilization rates. The y-axis shows the percentage of data (relative to the baseline AL framework) required to reach the different performance thresholds.

Classifier	Evaluation Metric	Standard	Oversampling	Proposed
DT	Accuracy	0.733 ± 0.092	0.732 ± 0.087	0.740 ± 0.087
DT	F-score	0.695 ± 0.088	0.698 ± 0.090	0.705 ± 0.092
DT	G-mean	0.804 ± 0.065	0.811 ± 0.060	0.816 ± 0.062
KNN	Accuracy	0.816 ± 0.091	0.818 ± 0.088	0.822 ± 0.091
KNN	F-score	0.775 ± 0.102	0.784 ± 0.108	0.788 ± 0.111
KNN	G-mean	0.852 ± 0.084	0.866 ± 0.072	0.869 ± 0.074
LR	Accuracy	0.802 ± 0.091	0.812 ± 0.088	0.821 ± 0.086
LR	F-score	0.749 ± 0.112	0.773 ± 0.116	0.784 ± 0.115
LR	G-mean	0.839 ± 0.093	0.870 ± 0.065	0.875 ± 0.064
RF	Accuracy	0.861 ± 0.076	0.861 ± 0.075	0.862 ± 0.077
RF	F-score	0.823 ± 0.105	0.827 ± 0.105	0.829 ± 0.105
RF	G-mean	0.886 ± 0.077	0.895 ± 0.063	0.895 ± 0.065

Table 4: Average AULC of each AL configuration tested. Each AULC score is calculated using the performance scores of each iteration in the validation set. By the end of the iterative process, each AL configuration used a maximum of 80% instances of the 60% instances that compose the training sets (*i.e.*, 48% of the entire preprocessed dataset).

(fully labeled training set, without AL) is shown in Table 6. The proposed AL method produces classifiers that are almost always able to outperform classifiers using the full training set (*i.e.*, the ones labeled as MP).

5.2. Statistical Analysis

When checking for statistical significance in a multiple dataset context it is important to account for the multiple comparison problem. Consequently, our statistical analysis focuses on the recommendations found in [47]. Overall, we perform 3 statistical tests. The Friedman test [48] is used to understand whether there is a statistically significant difference in performance between the 3 AL frameworks. As post hoc analysis, the Wilcoxon signed-rank test [49] was used to check for statistical significance between the performance of the proposed AL method and the oversampling AL method across datasets. As a second post hoc analysis, the Holm-Bonferroni [50] method was used to check for statistical significance between the methods using data generators and the Standard AL framework across classifiers and evaluation metrics.

G-mean Score	Classifier	Standard	Oversampling	Proposed
0.60	DT	3.2%	3.1%	3.2%
0.60	KNN	3.6%	2.6%	2.5%
0.60	LR	3.9%	2.2%	2.2%
0.60	RF	2.4%	2.1%	2.1%
0.66	DT	4.6%	4.6%	4.2%
0.66	KNN	4.9%	3.7%	3.5%
0.66	LR	5.7%	3.2%	3.1%
0.66	RF	3.0%	2.8%	2.7%
0.70	DT	6.6%	6.1%	5.8%
0.70	KNN	8.5%	5.0%	4.7%
0.70	LR	9.5%	4.6%	4.3%
0.70	RF	4.5%	3.2%	3.3%
0.76	DT	16.5%	13.0%	12.7%
0.76	KNN	17.8%	9.7%	9.0%
0.76	LR	16.6%	10.0%	7.8%
0.76	RF	10.1%	5.5%	5.5%
0.80	DT	36.1%	30.4%	27.1%
0.80	KNN	22.7%	18.0%	17.8%
0.80	LR	25.2%	16.0%	14.2%
0.80	RF	15.5%	9.0%	9.5%
0.86	DT	60.5%	56.7%	54.5%
0.86	KNN	39.9%	37.0%	37.8%
0.86	LR	32.6%	27.5%	27.0%
0.86	RF	28.0%	25.7%	25.7%
0.90	DT	72.5%	70.7%	67.8%
0.90	KNN	49.9%	50.3%	49.3%
0.90	LR	52.5%	53.8%	49.3%
0.90	RF	44.6%	42.6%	43.5%
0.96	DT	100.0%	99.5%	100.0%
0.96	KNN	79.4%	75.6%	71.6%
0.96	LR	87.5%	83.1%	79.8%
0.96	RF	63.6%	64.2%	63.1%

Table 5: Mean data utilization of AL algorithms, as a percentage of the training set.

Classifier	Evaluation Metric	MP	Standard	Oversampling	Proposed
DT	Accuracy	0.809 ± 0.086	0.802 ± 0.089	0.806 ± 0.089	0.812 ± 0.087
DT	F-score	0.774 ± 0.107	0.772 ± 0.096	0.775 ± 0.101	0.781 ± 0.103
DT	G-mean	0.853 ± 0.081	0.854 ± 0.069	0.860 ± 0.067	0.864 ± 0.068
KNN	Accuracy	0.882 ± 0.085	0.883 ± 0.087	0.877 ± 0.087	0.881 ± 0.093
KNN	F-score	0.848 ± 0.116	0.849 ± 0.115	0.847 ± 0.118	0.852 ± 0.121
KNN	G-mean	0.896 ± 0.094	0.899 ± 0.090	0.904 ± 0.078	0.907 ± 0.080
LR	Accuracy	0.855 ± 0.074	0.870 ± 0.073	0.858 ± 0.077	0.870 ± 0.076
LR	F-score	0.812 ± 0.113	0.835 ± 0.105	0.825 ± 0.106	0.838 ± 0.106
LR	G-mean	0.875 ± 0.099	0.895 ± 0.075	0.899 ± 0.059	0.907 ± 0.059
RF	Accuracy	0.897 ± 0.080	0.905 ± 0.078	0.904 ± 0.078	0.906 ± 0.077
RF	F-score	0.867 ± 0.107	0.877 ± 0.103	0.875 ± 0.108	0.877 ± 0.108
RF	G-mean	0.911 ± 0.081	0.917 ± 0.078	0.923 ± 0.067	0.925 ± 0.065

Table 6: Optimal classification scores. The Maximum Performance (MP) classification scores are calculated using classifiers trained using the entire training set.

486 Table 7 contains the *p-values* obtained with the Friedman test. The
487 difference in performance across AL frameworks is statistically significant at
488 a level of $\alpha = 0.05$ regardless of the classifier or evaluation metric being
489 considered.

Classifier	Evaluation Metric	p-value	Significance
DT	Accuracy	2.1e-17	True
DT	F-score	2.5e-24	True
DT	G-mean	2.8e-16	True
KNN	Accuracy	1.1e-46	True
KNN	F-score	1.8e-66	True
KNN	G-mean	6.4e-42	True
LR	Accuracy	9.9e-59	True
LR	F-score	2.0e-76	True
LR	G-mean	2.2e-59	True
RF	Accuracy	5.7e-42	True
RF	F-score	4.6e-55	True
RF	G-mean	1.3e-38	True

Table 7: Results for Friedman test. Statistical significance is tested at a level of $\alpha = 0.05$. The null hypothesis is that there is no difference in the classification outcome across oversamplers.

Table 8 contains the *p-values* obtained with the Wilcoxon signed-rank test. The proposed method was able to outperform both the standard AL framework, as well as the AL framework using a normal oversampling policy proposed in [18] with statistical significance in 9 out of 10 datasets.

The *p-values* shown in Table 9 refer to the results of the Holm-Bonferroni test. The proposed method’s superior performance was statistically significant for any combination of classifier and evaluation metric. Simultaneously, the proposed method established statistical significance in the 3 scenarios where the oversampling AL method failed to do so.

5.3. Discussion

In this paper, we study the application of data augmentation methods through the modification of the standard AL framework. This is done to further reduce the amount of labeled data required to produce a reliable classifier, at the expense of artificial data generation.

In Table 3 we found that the proposed method was able to outperform the Standard AL framework in all scenarios. The mean rankings are consistent with the mean AULC scores found in Table 4, while showing significant

Dataset	Oversampling	Standard
Baseball	5.0e-01	3.4e-01
Gas Drift	3.7e-26	4.6e-57
Image Segmentation	9.6e-18	2.1e-44
Japanese Vowels	2.4e-09	1.6e-32
Mfeat Zernike	1.2e-12	9.5e-40
Mice Protein	6.5e-32	1.5e-61
Pendigits	5.0e-18	2.3e-45
Texture	1.5e-22	6.7e-57
Vehicle	7.4e-11	7.9e-13
Waveform	8.9e-08	2.6e-02

Table 8: Adjusted p-values using the Wilcoxon signed-rank method. Bold values are statistically significant at a level of $\alpha = 0.05$. The null hypothesis is that the performance of the proposed framework is similar to that of the oversampling or standard framework.

Classifier	Evaluation Metric	Oversampling	Proposed
DT	Accuracy	4.5e-05	1.6e-10
DT	F-score	1.9e-07	2.7e-10
DT	G-mean	2.5e-06	3.1e-09
KNN	Accuracy	5.5e-02	1.1e-05
KNN	F-score	6.7e-11	6.3e-14
KNN	G-mean	8.3e-06	1.3e-07
LR	Accuracy	8.1e-02	3.4e-06
LR	F-score	7.1e-06	2.0e-20
LR	G-mean	2.2e-07	1.1e-11
RF	Accuracy	2.0e-01	2.8e-02
RF	F-score	2.2e-05	8.1e-07
RF	G-mean	2.0e-04	2.0e-04

Table 9: Adjusted p-values using the Holm-Bonferroni method. Bold values are statistically significant at a level of $\alpha = 0.05$. The null hypothesis is that the Oversampling or Proposed method does not perform better than the control method (Standard AL framework).

508 performance differences between the proposed method and both the stan-
509 dard and oversampling methods. The Friedman test in Table 7 showed that
510 the difference in the performance of these AL frameworks **are** statistically
511 significant, regardless of the classifier or performance metric being used.

512 The proposed method showed more consistent data utilization require-
513 ments to most of the assessed G-mean score thresholds when compared to
514 the remaining AL methods, as seen in Table 5. For example, to reach a G-
515 mean Score of 0.9 using the KNN and LR classifiers, the average amount of
516 data required with the Oversampling AL approach increased when compared
517 to the Standard approach. However, the proposed method was able to de-
518 crease the amount of data required in both situations. The robustness of the
519 Proposed method is clearer in Figure 6. In most cases, this method was able
520 **to** outperform the Oversampling method. At the same time, the proposed
521 method also addresses inconsistencies in situations where the Oversampling
522 method was unable to outperform the standard method.

523 The statistical analyses found in Tables 8 and 9 showed that the pro-
524 posed method’s superiority was statistically significant in all datasets except
525 one (Baseball) and established statistical significance when compared to the
526 Standard AL method for all combinations of classifier and performance met-
527 ric, including when the Oversampling AL method failed to do so. These
528 results show that the Proposed method increased the reliability of the new
529 AL framework and improved the quality of the final classifier while using less
530 data.

531 Even though it was not the core purpose of this study, we found that
532 the method proposed AL approach consistently outperformed the maximum
533 performance threshold. Specifically, in Table 6, the performance of the classi-
534 fiers originating from the proposed method was able to outperform classifiers
535 trained using the full training dataset in all 12 scenarios except one. This
536 suggests that the selection of a meaningful training subset training dataset
537 paired with data augmentation not only matches the classification perfor-
538 mance of ML algorithms, as it also improves them. Even in a setting with
539 fully labeled training data, the proposed method may be used as preprocess-
540 ing method to further optimize classification performance.

541 This study discussed the effect of data augmentation within the AL frame-
542 work, along with the exploration of optimal augmentation methods within
543 AL iterations. However, the conceptual nature of this study implies some
544 limitations. Specifically, the large **number** of experiments required to test
545 the method’s efficacy, along with the limited computational power available,

546 led to a limited exploration of the grid search’s potential. Future work should
 547 focus **on** understanding how the usage of a more comprehensive parameter
 548 tuning approach improves the quality of the AL method. In addition, the
 549 proposed method was not able to outperform the standard AL method **at**
 550 100% of scenarios. The exploration of other, more complex, data augmen-
 551 tation techniques might further improve its performance through the pro-
 552 duction of more meaningful training observations. Specifically, in this study
 553 we assume that all datasets used follow a manifold, allowing the usage of
 554 G-SMOTE as a data augmentation approach. However, this method cannot
 555 be used **in** more complex, non-euclidean spaces. In this scenario, the usage
 556 of G-SMOTE is not valid and might lead to the production of noisy data.
 557 Deep Learning-based data augmentation techniques are able to address this
 558 limitation and improve the overall quality of the artificial data being gener-
 559 ated. We also found significant standard errors throughout our experimental
 560 results (see Subsection 5.1), which is consistent with the findings in [18, 42].
 561 This suggests that the usage of more robust generators did not decrease the
 562 standard error of AL performance. Instead, AL’s performance variability is
 563 likely dependent on the quality of its initialization.

564 **6. Conclusion**

565
 566 The ability of training ML classifiers is usually limited to the availability
 567 of labeled data. However, manually labeling data is often expensive, which
 568 makes the usage of AL particularly appealing to select the most informative
 569 observations and reduce the amount of required labeled data. On the other
 570 hand, the introduction of data variability in the training dataset can also be
 571 done via data augmentation. However, most, if not all, AL configurations us-
 572 ing some form **of** data augmentation are domain and/or task-specific. These
 573 methods typically **apply** deep learning approaches **to** both classification and
 574 data augmentation. Consequently, they may not be applicable for other
 575 classification tasks or when the available computational power is insufficient.

576 In this paper, we proposed a domain-agnostic AL framework that im-
 577 plements Data Augmentation and hyperparameter tuning. We found that
 578 a heuristic Data Augmentation algorithm is sufficient to improve the data
 579 selection efficiency in AL. Specifically, the data augmentation method used
 580 almost always increased AL performance, regardless of the target goal (*i.e.*,
 581 optimizing classification or data selection efficiency). The usage of data aug-

582 mentation reduced the number of iterations required to train a classifier with
583 a performance as good as (or better than) classifiers trained with the entire
584 training dataset (*i.e.*, without using AL). In addition, the proposed method
585 reduced the size of the training dataset, which is expanded with artificial
586 data.

587 With this AL configuration, data selection in AL iterations aims towards
588 observations that optimize the quality of the artificial data produced. The
589 substitution of less informative labeled data with artificial data is especially
590 useful in this context, since it allows the reduction of some of the user interac-
591 tion necessary to reach a sufficiently informative dataset. In order to further
592 improve the proposed method future work will (1) focus on the development
593 of methods with varying data augmentation policies depending on the differ-
594 ent input space regions, (2) develop augmentation-sensitive query functions
595 capable of avoiding the unnecessary selection of similar observations from the
596 unlabeled dataset and (3) better understand the gap between heuristic/input
597 space data augmentation techniques and neural network/feature space data
598 augmentation techniques in an AL context.

599 Declarations

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604 PCIF/SSI/0102/2017.

605 *Code availability*

606 The analyses and source code is available at [github.com/joaopfonseca/ml-](https://github.com/joaopfonseca/ml-research)
607 [research](https://github.com/joaopfonseca/ml-research).

608 References

- 609 [1] V. Nath, D. Yang, B. A. Landman, D. Xu, H. R. Roth, Diminishing
610 uncertainty within the training pool: Active learning for medical image
611 segmentation, *IEEE Transactions on Medical Imaging* 40 (10) (2021)
612 2534–2547.

- [2] Y. Sverchkov, M. Craven, A review of active learning approaches to experimental design for uncovering biological networks, *PLoS Computational Biology* 13 (2017) e1005466.
- [3] X. Li, D. Kuang, C. X. Ling, Active learning for hierarchical text classification, *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)* 7301 LNAI (2012) 14–25.
- [4] Y. Li, J. Yin, L. Chen, Seal: Semisupervised adversarial active learning on attributed graphs, *IEEE Transactions on Neural Networks and Learning Systems* 32 (7) (2021) 3136–3147.
- [5] O. Siméoni, M. Budnik, Y. Avrithis, G. Gravier, Rethinking deep active learning: Using unlabeled data at model training, *Proceedings - International Conference on Pattern Recognition* (2020) 1220–1227.
- [6] J. E. Van Engelen, H. H. Hoos, A survey on semi-supervised learning, *Machine Learning* 109 (2) (2020) 373–440.
- [7] O. Sener, S. Savarese, Active learning for convolutional neural networks: A core-set approach, in: *International Conference on Learning Representations*, 2018.
- [8] Y. Leng, X. Xu, G. Qi, Combining active learning and semi-supervised learning to construct svm classifier, *Knowledge-Based Systems* 44 (2013) 121–131.
- [9] H. Yu, X. Yang, S. Zheng, C. Sun, Active learning from imbalanced data: A solution of online weighted extreme learning machine, *IEEE Transactions on Neural Networks and Learning Systems* 30 (2019) 1088–1103.
- [10] W. Zong, G.-B. Huang, Y. Chen, Weighted extreme learning machine for imbalance learning, *Neurocomputing* 101 (2013) 229–242.
- [11] J. Qin, C. Wang, Q. Zou, Y. Sun, B. Chen, Active learning with extreme learning machine for online imbalanced multiclass classification, *Knowledge-Based Systems* 231 (2021) 107385.

- 643 [12] W. Liu, H. Zhang, Z. Ding, Q. Liu, C. Zhu, A comprehensive active
644 learning method for multiclass imbalanced data streams with concept
645 drift, *Knowledge-Based Systems* 215 (2021) 106778.
- 646 [13] A. Tharwat, W. Schenck, Balancing exploration and exploitation: A
647 novel active learner for imbalanced data, *Knowledge-Based Systems* 210
648 (2020) 106500.
- 649 [14] Y.-Y. Kim, K. Song, J. Jang, I.-c. Moon, Lada: Look-ahead data ac-
650 quisition via augmentation for deep active learning, *Advances in Neural*
651 *Information Processing Systems* 34 (2021).
- 652 [15] G. Douzas, F. Bacao, Geometric SMOTE a geometrically enhanced
653 drop-in replacement for SMOTE, *Information Sciences* 501 (2019) 118–
654 135.
- 655 [16] J. Katz-Samuels, J. Zhang, L. Jain, K. Jamieson, Improved algorithms
656 for agnostic pool-based active classification, in: *International Conference*
657 *on Machine Learning*, PMLR, 2021, pp. 5334–5344.
- 658 [17] T. Su, S. Zhang, T. Liu, Multi-spectral image classification based on an
659 object-based active learning approach, *Remote Sensing* 12 (2020) 504.
- 660 [18] J. Fonseca, G. Douzas, F. Bacao, Increasing the Effectiveness of Active
661 Learning: Introducing Artificial Data Generation in Active Learning
662 for Land Use/Land Cover Classification, *Remote Sensing* 2021, Vol. 13,
663 Page 2619 13 (13) (2021) 2619.
- 664 [19] D. Yoo, I. S. Kweon, Learning loss for active learning, in: *Proceedings*
665 *of the IEEE/CVF Conference on Computer Vision and Pattern Recog-*
666 *nition*, 2019, pp. 93–102.
- 667 [20] H. H. Aghdam, A. Gonzalez-Garcia, A. Lopez, J. Weijer, Active learn-
668 ing for deep detection neural networks, in: *Proceedings of the IEEE*
669 *International Conference on Computer Vision*, Vol. 2019-Octob, 2019,
670 pp. 3671–3679.
- 671 [21] B. Gu, Z. Zhai, C. Deng, H. Huang, Efficient active learning by querying
672 discriminative and representative samples and fully exploiting unlabeled
673 data, *IEEE Transactions on Neural Networks and Learning Systems* 32
674 (2021) 4111–4122.

- [22] P. Kumar, A. Gupta, Active learning query strategies for classification, regression, and clustering: A survey, *Journal of Computer Science and Technology* 2020 35:4 35 (2020) 913–945.
- [23] Y. Fu, X. Zhu, B. Li, A survey on instance selection for active learning, *Knowledge and information systems* 35 (2) (2013) 249–283.
- [24] S. Behpour, K. M. Kitani, B. D. Ziebart, Ada: Adversarial data augmentation for object detection, *Proceedings - 2019 IEEE Winter Conference on Applications of Computer Vision, WACV 2019* (2019) 1243–1252.
- [25] Z. Zhong, L. Zheng, G. Kang, S. Li, Y. Yang, Random erasing data augmentation, in: *Proceedings of the AAAI Conference on Artificial Intelligence*, Vol. 34, 2020, pp. 13001–13008.
- [26] T. DeVries, G. W. Taylor, Dataset augmentation in feature space, in: *5th International Conference on Learning Representations, ICLR 2017 - Workshop Track Proceedings, International Conference on Learning Representations, ICLR, 2017*.
- [27] C. Shorten, T. M. Khoshgoftaar, A survey on image data augmentation for deep learning, *Journal of Big Data* 6 (1) (2019) 1–48.
- [28] O. Kashefi, R. Hwa, Quantifying the evaluation of heuristic methods for textual data augmentation, in: *Proceedings of the Sixth Workshop on Noisy User-generated Text (W-NUT 2020)*, Association for Computational Linguistics, Online, 2020, pp. 200–208.
- [29] T. Tran, T.-T. Do, I. Reid, G. Carneiro, Bayesian generative active deep learning, in: *International Conference on Machine Learning*, PMLR, 2019, pp. 6295–6304.
- [30] S. Sinha, S. Ebrahimi, T. Darrell, Variational adversarial active learning, in: *Proceedings of the IEEE/CVF International Conference on Computer Vision*, 2019, pp. 5972–5981.
- [31] K. Kim, D. Park, K. I. Kim, S. Y. Chun, Task-aware variational adversarial active learning, in: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, 2021, pp. 8166–8175.

- 705 [32] Y. Ma, S. Lu, E. Xu, T. Yu, L. Zhou, Combining active learning and
706 data augmentation for image classification, in: Proceedings of the 2020
707 3rd International Conference on Big Data Technologies, 2020, pp. 58–62.
- 708 [33] H. Quteineh, S. Samothrakis, R. Sutcliffe, Textual data augmentation
709 for efficient active learning on tiny datasets, in: Proceedings of the
710 2020 Conference on Empirical Methods in Natural Language Processing
711 (EMNLP), 2020, pp. 7400–7410.
- 712 [34] Q. Li, Z. Huang, Y. Dou, Z. Zhang, A framework of data augmentation
713 while active learning for chinese named entity recognition, in: Interna-
714 tional Conference on Knowledge Science, Engineering and Management,
715 Springer, 2021, pp. 88–100.
- 716 [35] C. Wu, The decision tree approach to classification., Purdue University,
717 1975.
- 718 [36] T. Cover, P. Hart, Nearest neighbor pattern classification, IEEE Trans-
719 actions on Information Theory 13 (1) (1967) 21–27.
- 720 [37] T. K. Ho, Random decision forests, in: Proceedings of the Third Inter-
721 national Conference on Document Analysis and Recognition (Volume 1)
722 - Volume 1, ICDAR '95, IEEE Computer Society, USA, 1995, p. 278.
- 723 [38] J. A. Nelder, R. W. Wedderburn, Generalized linear models, Journal of
724 the Royal Statistical Society: Series A (General) 135 (3) (1972) 370–384.
- 725 [39] L. A. Jeni, J. F. Cohn, F. De La Torre, Facing imbalanced data - Recom-
726 mendations for the use of performance metrics, in: Proceedings - 2013
727 Humaine Association Conference on Affective Computing and Intelligent
728 Interaction, ACII 2013, 2013, pp. 245–251.
- 729 [40] M. Fatourechi, R. K. Ward, S. G. Mason, J. Huggins, A. Schloegl, G. E.
730 Birch, Comparison of evaluation metrics in classification applications
731 with imbalanced datasets, in: 2008 seventh international conference on
732 machine learning and applications, IEEE, 2008, pp. 777–782.
- 733 [41] M. Kubat, S. Matwin, et al., Addressing the curse of imbalanced training
734 sets: one-sided selection, in: Icml, Vol. 97, Citeseer, 1997, pp. 179–186.

- 735 [42] D. Kottke, A. Calma, D. Huseljic, G. Kreml, B. Sick, Challenges of
736 reliable, realistic and comparable active learning evaluation, in: CEUR
737 Workshop Proceedings, Vol. 1924, 2017, pp. 2–14.
- 738 [43] T. Reitmaier, B. Sick, Let us know your decision: Pool-based active
739 training of a generative classifier with the selection strategy 4ds, Infor-
740 mation Sciences 230 (2013) 106–131.
- 741 [44] J.-F. Kagy, T. Kayadelen, J. Ma, A. Rostamizadeh, J. Strnadova, The
742 practical challenges of active learning: Lessons learned from live exper-
743 imentation, arXiv preprint arXiv:1907.00038 (6 2019).
- 744 [45] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion,
745 O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vander-
746 plas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, É. Duchesnay,
747 Scikit-learn: Machine Learning in Python, Journal of Machine Learning
748 Research 12 (Oct) (2011) 2825–2830.
- 749 [46] G. Lemaître, F. Nogueira, C. K. Aridas, Imbalanced-learn: A python
750 toolbox to tackle the curse of imbalanced datasets in machine learning,
751 Journal of Machine Learning Research 18 (17) (2017) 1–5.
- 752 [47] J. Demšar, Statistical comparisons of classifiers over multiple data sets,
753 Journal of Machine Learning Research 7 (2006) 1–30.
- 754 [48] M. Friedman, The use of ranks to avoid the assumption of normality
755 implicit in the analysis of variance, Journal of the american statistical
756 association 32 (200) (1937) 675–701.
- 757 [49] F. Wilcoxon, Individual Comparisons by Ranking Methods, Biometrics
758 Bulletin 1 (6) (1945) 80.
- 759 [50] S. Holm, A simple sequentially rejective multiple test procedure, Scan-
760 dinavian journal of statistics (1979) 65–70.