Regularization Oversampling for Classification Tasks: To Exploit What You Do Not Know

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Abstract

In numerous binary classification tasks, the two groups of instances are not equally represented, which often implies that the training data lacks sufficient information to model the minority class correctly. Further, many traditional classification models make arbitrarily overconfident predictions outside the range of the training data. The above mentioned issues severely impact the deployment and usefulness of these models in real life. In this paper, we propose the Boundary Regularizing Out-Of-Distribution (BROOD) sampler that adds artificial data points on the edge of the training data. By exploiting these artificial samples, we are able to regularize the decision surface of discriminative machine learning models and make more prudent predictions. Next, it is crucial to correctly classify many positive instances in a limited pool of instances one can investigate with the available resources. By smartly assigning predetermined non-uniform class probabilities outside the training data, we can emphasize certain data regions and improve classifier performance on various material classification metrics. The good performance of the proposed methodology is illustrated in a case study that consists of both benchmark balanced and imbalanced classification data sets.

Keywords: Binary classification, Regularization, Sampling, Data imbalance

1. Introduction

The classification of instances into two groups is one of the core concepts of data mining. Often, a major challenge arises because the two classes are not equally represented. For instance, the imbalance is often present in fraud [1], customer churn [61], credit scoring [38] and bankruptcy [52] data sets. Many traditional machine learning models try to minimize the overall error, which causes the machine learning model to focus on the majority (negative) class which usually results in a poor capability to find minority (positive) class samples. Hence, machine learning models could achieve excellent accuracy without detecting any positive cases by training on imbalanced data sets. Unfortunately, the detection of minority samples is often of utmost importance. For example, in fraud applications, severe financial and credibility losses are incurred if one is not able to detect the fraudulent instances. The authors of [11] and [61] define several categories to deal with these imbalanced data sets. First, one can design new or modify existing algorithms to handle the class imbalance issue. For instance, some methods try to assign a cost to specific data points to emphasize their importance or in an attempt to mimic reality. For instance, papers like [42], [3], and [2] use and develop cost-sensitive learning methods which account for different costs of misclassification. Next, ensemble classifiers have also been shown to mitigate the imbalance issue. A good summary of ensemble learning algorithms tailored to learn from imbalanced data sets can be found in [16].

Finally, one can modify the provided training data as a preprocessing step by decreasing the number of majority samples or increasing the number of minority samples. In general, it is believed that oversampling is more effective than undersampling [17]. The most famous oversampling technique is SMOTE [8] and has been shown to improve performance in many applications. To give some examples, the authors of [52] show that oversampling methods can enhance bankruptcy prediction performance in case of data imbalance. Similarly, in [35], one exploits SMOTE to investigate weaknesses in internal control databases and handle the appurtenant data imbalance issue. In this paper, we also develop an oversampling algorithm. However, we do not create artificial samples that belong to the minority class, but our method samples artificial data points on the boundary of the data set that can be exploited during the training phase.

Next, machine learning models have proven that they can achieve satisfactory performance predicting test samples simi-

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lar to the training data. However, machine learning models tend to be overconfident in data regions they have never seen before [27], [26], and [31]. This random behaviour in the presence of dissimilar or unseen data implies that developing and deploying machine learning models in real life is very challenging. To tackle learning on non-stationary data, one can rely on techniques that can handle concept drift [56]

Further, if only a limited number of minority instances are available, it is hard for the model to classify positive data instances dissimilar to the training data correctly. To tackle this issue, one can address techniques that enable smart querying, like active learning [44]. Furthermore, if the minority class is poorly defined, one can use one-class classification [23]. To find new or outlying constructions, one can rely on novelty/anomaly detection [39] techniques.

In this paper, we propose the Boundary Regularizing Out-Of-Distribution (BROOD) sampler that adds artificial data points on the data distribution's boundary to aid the machine learning model in learning a suitable decision surface. By exploiting these artificial samples, we are able to regularize the decision surface of discriminative machine learning models and make more reliable predictions. This yields more interpretable machine learning models that exploit the assignment of high or low probabilities in Out-Of-Distribution (OOD) regions.

Using the Discounted Cumulative Gain (DCG) metric, we show that our approach has a substantial positive effect on detecting minority instances when only limited sources are available. Further, we show that our approach positively affects other performance metrics like the Average Precision (AP). In particular, we

- propose the Boundary Regularising Out-Of-Distribution (BROOD) sampler that samples artificial data points that lie on the data distribution's boundary;
- investigate if one can use artificial samples to regularize the decision surface of various machine learning models;
- elucidate the difference between existing oversampling approaches and show how our methodology can complement minority oversampling methods;
- illustrate the excellent performance of the proposed sampler in an extensive data study by using the XGBoost [9] algorithm.

The data study consists of various balanced and imbalanced classification data sets. Further, we focus on the XGBoost algorithm, which is considered one of the best algorithms to learn from tabular data.

2. Literature Review

2.1. Artificial Minority Sampling

If the data set is imbalanced, traditional machine learning models will only learn the specific data regions where the minority samples are present, which may have a negative impact on the predictive power. Moreover, due to this class imbalance, traditional classification models tend to be biased towards the majority class. An extensive summary of methods to mitigate the class imbalance problem can be found in [61].

One possible procedure is to assign additional weights on minority class instances (or to replicate the instance multiple times) to enhance their importance. However, this approach can result in severe over-fitting. A way to mitigate this issue is to apply an oversampling technique. For instance, the conventional SMOTE [8] generates similar synthetic samples of the minority class ~~to cover more broad data regions.~~ by sampling artificial data points on a straight line between the minority classes' nearest neighbors. ~~to achieve this~~This aids the classifier in building larger decision regions enclosing nearby actual and artificial minority class points and reduces its bias introduced by the class imbalance.

~~A well-known extension of SMOTE is Borderline SMOTE [21], where only minority samples near the class boundary are oversampled. Another famous extension~~A well-known extension of SMOTE is ADASYN [22]. ADASYN ~~is less extreme than Borderline SMOTE as it~~ generates synthetic samples from minority instances proportional to the impurity of the instance's neighborhood. This approach aims to shift the decision boundary by letting the classifier focus more on the difficult-to-learn minority instances. A weakness of ADASYN is that this method emphasizes the importance of noisy minority instances and outliers.

Next, ROSE [32] is a popular oversampling technique that generates data from a class-dependent kernel density estimate [7] with a certain smoothing matrix. ~~that defines a neighborhood of the existing samples and generates additional artificial samples in this neighborhood.~~ By exploiting the extensive kernel density estimation literature, one is able to choose suitable smoothing matrices. Furthermore, ROSE can be used as smoothed bootstrap resampling technique and thus has applications in bootstrap aggregating (bagging) procedures.

Although synthetic oversampling techniques reduce overfitting by creating similar artificial minority samples, always keep in mind that many standard oversampling techniques introduce noise in the data set and enhance class overlap.

~~Many other methodological papers propose new oversampling techniques to enhance performance after training an initial machine learning model. For instance, in [25] one tries to mitigate the imbalance problem by developing an oversampling technique, denoted M-SMOTE, that exploits misclassified minority samples from a Gaussian process classifier. One shows that the M-SMOTE algorithm performs better than SMOTE on various performance metrics. Similarly, the authors of [40] train a support vector machine and create additional samples in the space of the minority data points closest to the support vector machine's decision boundary. The authors show superior performance compared to the performance of various samplers.~~

Recently, new methods to mitigate the introduction of noise have been proposed. For instance, the authors of [12] uses K-means clustering to discover clusters with a high ratio of minority instances. ~~sparse and pure areas of minority samples~~ Artificial data points are only sampled, using SMOTE, in these data areas as it avoids noise generation and data overlap. More-

over, one is also able to improve within-class imbalance by assigning more synthetic samples to clusters with a high average distance among the cluster's minority samples. The authors show that their method outperforms various minority oversamplers. Likewise, to reduce data overlap while generating artificial samples, the authors of [49] first train a Support Vector Data Description (SVDD) model [50] to define overlapping instances which will be removed during the generation of minority samples. Furthermore, the authors address hard-to-learn and within-class imbalance issues by constructing boundary and density factors. These factors enable the creation of more artificial samples from minority instances, using SMOTE, in low-density regions and regions close to the SVDD class boundary. The authors show superior performance compared to the performance of various samplers. Of course, these methods have an additional layer of complexity as one needs to train an initial machine learning model like K-means or a SVDD model.

An important property of OOD samplers is that properly generated OOD samples should also not introduce noise and data overlap. We give an overview of existing OOD samplers in the next subsection.

2.2. Out-Of-Distribution Sampling

Let us introduce some notation. We denote with $\boldsymbol{x}$ the data attributes and with y the actual response of an instance. The symbol ∂ represents a boundary, and $\boldsymbol{\theta}$ represents the model's hyper-parameters.

Most discriminative machine learning models are overconfident in unseen data regions as no data is available to guide the model. One can train generative classifiers to solve this issue as these models also incorporate data distributions. Generative classifiers model the joint probability $P(X, Y)$ from which we can derive $P(Y|X)$. However, these classifiers often make stronger modeling assumptions and are overtaken by discriminative models for large sample sizes [36].

Another approach to bypass this problem is by first detecting the OOD data points and only using the trained model to predict the In-Distribution (ID) data points. To detect these OOD samples, one can train anomaly detection models like Isolation Forests (IF) [28] or one-class classification models like SVDD on the training data set. However, this method is unsatisfactory as one cannot obtain predictions of the OOD data's label by using this method.

In the fields of open set recognition [19] (train classifiers that can classify seen classes and deal with unseen classes) and OOD detection [59] (detect test samples drawn from a distribution that is different from the training distribution), one proposes various oversampling techniques tackling issues that arise due to unseen data. In [26], one trains deep neural networks (NNs) more conservatively by exposing the neural classification networks to OOD samples. Denote with f_{id} and with f_{ood} the ID and OOD data distributions, respectively. One proposes to minimize

$$L(X, \boldsymbol{y}, \boldsymbol{\theta}) = \mathbb{E}_{f_{id}}\left[P_{\boldsymbol{\theta}}(y|\boldsymbol{x})\right] + \lambda \mathbb{E}_{f_{ood}}\left[KL(\mathcal{U}(y)||P_{\boldsymbol{\theta}}(y|\boldsymbol{x}))\right] \quad (1)$$

with $\mathcal{U}(y)$ the uniform distribution. This causes the classifier to assign the base value (the class prior) to the OOD samples. As it is infeasible to sample the whole OOD space, one decides to sample OOD samples close to the ID data points. In this paper, one constructs a Generative Adversarial Network (GAN) [20] to generate OOD samples. The discriminator is trained to distinguish between artificiality-generated samples and ID data points. The generator is trained to fool the discriminator (generate samples close to the ID data points) and ~~one imposes an additional term to penalize the generator if it generates samples with a high KL divergence with the uniform distribution to ensure that~~ to generate low-density artificial samples. The classifier is trained by minimizing equation 1. A limitation is that one imposes the same class prior to all the OOD samples. The three models are trained in an alternating manner. The authors show their method's effectiveness using deep convolutional NNs on image data sets by comparing their method to a baseline detector. Furthermore, the authors show that the OOD samples can also handle unseen classes by learning an OOD class. Similarly, the authors of [60] generate ID and OOD samples in an unsupervised manner using a GAN. They exploit these samples to distinguish between all seen and potential unseen classes employing Support Vector Machines (SVMs) with a Radial Basis Function (RBF) kernel. They show effectiveness on toy, image and document classification data sets by comparing their method to various methods for open-set recognition. Likewise, in [18], one generates OOD samples using a GAN, incorporating the ability to deal with unknown classes using extreme value theory. The authors use NNs and show the model's usefulness in image classification tasks by comparing their method to baseline detectors without generating artificial samples.

In [53], one uses a Conditional Variational Auto Encoder (CVAE) [24], distinguishing between two types of OOD samples surrounding the latent encoding and exploiting the OOD samples for OOD detection. The authors compare their model to other classifier-based OOD detectors on image classification data sets using NNs. Although GANs and (V)AEs are good tools for generating data, they are often challenging to train.

In [33], one proposes an approach to sample data points close to the ID data set without the explicit need to use a GAN or (V)AE. The authors state that the data sampled by this method can be used to safeguard NNs and validate generalization performance. To create a suitable artificial sample, one randomly selects a data point from the ID data set and iteratively moves (starting from the data point) in a random direction. If the minimum distance between the new location and the ID data is satisfactory, the iteration stops, and one has sampled one OOD sample. The authors also include a 'softness' possibility to stop iterating even if the minimum distance is not achieved. Especially for high-dimensional data, it is difficult to assign a suitable minimum distance and step size. The authors use a VAE to construct a low-dimensional data embedding in their experiments. Further, the approach is relatively slow and very local in nature as the algorithm samples one artificial instance at a time by creating random directions from a random ID data point. Next, fewer artificial OOD samples will be sampled in sparse

data regions as one samples from a random ID data point. The authors show that their method is able to improve OOD detection on image data and provide a case study on the synthetic generation of OOD trajectories for automated driving. Nevertheless, to our knowledge, no previous research has been done that provides comparisons and discusses the limitations of existing OOD samplers.

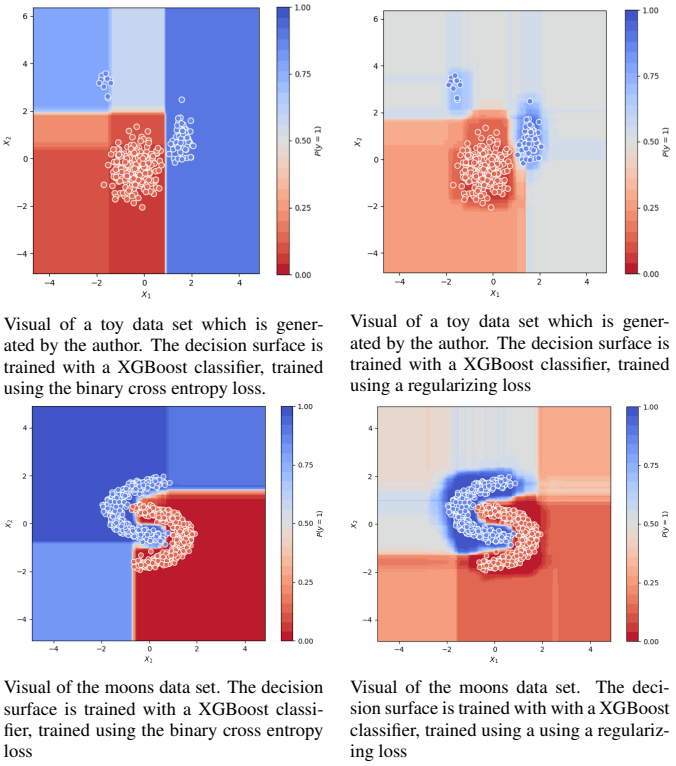
We propose a computationally attractive OOD sampler that mitigates the previously mentioned problems without needing GANs or (V)AEs, enabling us to assign class-specific probabilities outside the training data.

2.3. *Research Questions*

As no data is available to guide the model due to insufficient training data or concept drift, discriminative machine learning models assign arbitrarily overconfident predictions to this data. This is an important problem as it causes people to lose confidence in the model as the predictions are not substantiated.

Hence, machine learning models should be able to assign a pre-determined probability to data regions it has never seen before. Consider the case where one only has the resources to investigate a limited number of data instances. If one assigns low probabilities to unseen data regions, these regions will not be important, and one will exploit the current knowledge of training data. Conversely, if one assigns high probabilities to unseen data regions, these regions are important, and one will be encouraged to investigate these new data regions.

Figure 1 visualizes the decision boundary of XGBoost [9] classifiers on a toy data set created by the author and the well-known moons data set. On the left-hand side, we plot the decision boundary of the XGBoost classifier, which is trained using the binary cross entropy loss. One can deduce that this classifier is arbitrarily confident in certain data regions. For instance, the model assigns an unfounded high probability in the lower right corner for the toy data set.



Visual of a toy data set which is generated by the author. The decision surface is trained with a XGBoost classifier, trained using the binary cross entropy loss.

Visual of a toy data set which is generated by the author. The decision surface is trained with a XGBoost classifier, trained using a regularizing loss

Visual of the moons data set. The decision surface is trained with a XGBoost classifier, trained using the binary cross entropy loss

Visual of the moons data set. The decision surface is trained with with a XGBoost classifier, trained using a using a regularizing loss

Figure 1: Visual comparison of various decision surfaces. On the left-hand side we plot the decision surfaces that are trained with the XGBoost classifier using the standard binary cross-entropy loss. On the right-hand side we plot the decision surfaces that are trained with the XGBoost classifier using a regularizing loss.

We aim to construct decision surfaces like those on the right-hand side. The classifier should assign, in general, a high probability to the ID minority sample regions and a low probability to the ID majority sample regions. Next, pre-determined probabilities should be assigned to the OOD data regions 'close' to the ID minority data points and far from the ID majority data points. Further, one should be able to assign pre-determined probabilities to the OOD regions 'far' from the ID minority samples and 'close' to the ID majority samples. For the plots on the right-hand side of figure 1, OOD data regions closer to the ID minority samples have a higher probability relative to the data regions closer to the ID majority samples.

We aim to create artificial samples on the boundary of the training data distribution and the minority/majority class that will guide our model in unseen data regions. More rigorously, for all responses y, we create samples on $\partial\hat{P}(X|Y = y) \cap \partial\hat{P}(X)$, defining the class-specific boundary between ID and OOD data. Thus, we investigate the following research questions:

RQ1: Are artificial OOD samples able to suitably regularize the machine learning model's probability boundary?

RQ2: Are artificial OOD samples able to enhance the machine learning model's performance? Does our approach complement existing minority oversampling methods?

RQ3: What are the additional advantages of artificial OOD

samples for imbalanced classification tasks?

From the previous discussion, if new data points lie in a data region where there is no or only a little information available, we believe that the inclusion of artificial OOD samples positively impacts the predictive power of machine learning models. Further, suppose the training data captures all data regions present in the test data. In that case, we expect that the inclusion of artificial OOD samples will not have a negative impact on the performance measures as these samples will not interfere with the ID data points.

3. Methodology

In this section, we first develop a new oversampling technique that can efficiently generate artificial OOD samples. Next, we elucidate how we can use these artificial samples to regularise machine learning models in data regions it has never seen before. Finally, we discuss how the sampler's hyper-parameters affect the samples generated.

3.1. Boundary Regularizing Out-Of-Distribution (BROOD) Sampling

In order to answer the research questions, we need to construct a suitable OOD sampler. We name our sampler the Boundary Regularising Out-Of-Distribution (BROOD) sampler since we construct a sampler that creates artificial data points at the boundary of the training data to regularize the decision surfaces of machine learning models. As properly generated BROOD samples are situated on the edge of the training data, they should not introduce noise. We divide the BROOD sampler's pseudo-code 1 into six steps. In the following paragraphs, we substantiate the BROOD sampler's different steps, discuss its helper functions, and elaborate on its five input parameters.

In the first three steps, we calculate preliminary results that we exploit in the last three steps. In the first step, we quantify data dispersion, enabling us to construct artificial samples at a suitable distance from the ID points in the last three steps. Moreover, we determine the data points from which we will sample in the first step. In the second step, we construct directions that we address in the future to create artificial OOD samples. In the third step, we determine the relevant neighborhoods of the ID data points from which we will sample. We will use these neighbors to efficiently determine potential artificial samples that could interfere with the ID data points. The first three steps are all executed once.

In the fourth step, we query a data point and find the attributes of the instances that belong to the relevant neighborhoods of this data point. In the fifth step, we create artificial OOD samples using the previously constructed directions and delete OOD samples that lie too close to the ID data points and OOD samples of the same label. The artificial OOD samples get the same label as the point from which they are sampled. In the last step, we update the neighborhoods with the retained OOD samples to enhance sparseness and reduce duplicates.

The BROOD sampler makes use of several helper functions. In algorithm 2, one finds the pseudo-code to construct scalers related to data dispersion. Next, in algorithm 3, one finds the pseudo-code of the function that samples points on a sphere and creates directions. In algorithm 4, one finds the pseudo-code to calculate Mahalanobis distances. Finally, one can find the pseudo-code to appropriately scale the directions in algorithm 5.

The first prominent input parameter of the BROOD sampler is h_{strat}. It is infeasible to sample data that cover the whole potential OOD data space. Hence, we aim to generate artificial samples that are far enough (but not too far) from the original ID samples. Thus, one must choose a suitable distance between the original data and the artificial samples. We use the extensive literature on kernel density estimation to achieve this [7]. Kernel density estimation is a non-parametric way to estimate the probability density function of a particular random variable. For this task, one chooses a suitable bandwidth that balances both bias and variance of the density estimate. Let us introduce some notation. We denote with h_i and σ_i the bandwidth and the standard deviation that correspond with dimension i, respectively. Next, we denote with d the number of dimensions and with $H = \text{diag}(h_1^2, \ldots, h_d^2)$ a matrix of squared bandwidths. By optimizing the asymptotic mean integrated squared error, under normality of the data and a Gaussian kernel function, one can derive the rule of thumb selector [7] that is given by

$$\hat{h}_i = \left(\frac{4}{d+2}\right)^{\frac{1}{d+4}} n^{\frac{-1}{d+4}} \sigma_i. \tag{2}$$

We use this bandwidth to obtain a grasp of the dispersion of the data over different dimensions. Recall that we are not interested in estimating the actual densities accurately. One can also use a label-dependent version of the rule of thumb selector like in ROSE [32], which did not cause a substantial performance increase in our experiments.

Although the (class-dependent) rule of thumb selector is often satisfactory, this choice can suffer from non-constant density regions in the feature space as $\hat{\boldsymbol{h}}$ is not instance dependent. Hence, we provide a dispersion measure with an instance dependent $\hat{\boldsymbol{h}}$ according to the sparseness of data regions. Denote with d_{j_k} the Euclidean distance from an instance $\boldsymbol{x}_j$ to its k-nearest neighbor and with n_{j_k} the set of k-nearest neighbors of instance $\boldsymbol{x}_j$. In [6], one proposes to use d_{j_k} as bandwidth for kernel density estimation. Since outliers have a substantially higher d_{j_k}, we decide to use local density information of the k-nearest neighbors. Hence, instead of using the k-nearest neighbor distance of the instance itself, we take the mean of the k-nearest neighbor distance of the instance's neighbors. Notice the strong connection with (simple) local factor outlying [43]. In this case, we define $\hat{\boldsymbol{h}}$ as

$$\hat{\boldsymbol{h}}(\boldsymbol{x}_j) = \sum_{\boldsymbol{x}_i \in n_{j\_k}} d_{i\_k}. \tag{3}$$

One disadvantage of this approach is that we need to define one additional hyper-parameter k. We do not claim that we propose an optimal $\hat{\boldsymbol{h}}$ and many other choices are possible.

Under the assumption that $\hat{H}$ is positive definite, we find that

$$\hat{H}^{-1} = \text{diag}\left(1/\hat{h}_1^2, \ldots, 1/\hat{h}_d^2\right). \quad (4)$$

The Mahalanobis distance between two points p_1, p_2 with covariance matrix $\hat{H}$ equals

$$d_{(\text{mahal},\hat{H})}(p_1, p_2) = \sqrt{(p_1 - p_2)\hat{H}^{-1}(p_1 - p_2)}. \quad (5)$$

The next crucial input parameter of the BROOD sampler is $\text{query}_{\text{strat}}$. We use this parameter in the first step as this parameter determines the ID data points we will utilize to sample artificial data points. The queried data points can be chosen randomly, by their class, or by an OOD detector like IF [28] or SVDD [50].

The parameter $n_{\text{dir\_max}}$ is used in the second step and represents the maximal number of directions (and thus potential new artificial data points) which we will sample at each queried ID data point. We create directions by sampling points on the surface of a d-dimensional hypersphere. To generate one direction, we sample a vector $\boldsymbol{v}$ from a standard normal distributed ($\boldsymbol{v} \sim \mathcal{N}(\mathbf{0}, I_d)$) [46] and scale this vector accordingly such that the norm of $\boldsymbol{v}$ is equal to one. By executing this procedure multiple times, we can randomly sample points on the surface of a d-dimensional hypersphere. Notice that we use these directions for every point we will sample from, as this has a significant positive effect on computation time.

Next, we want the directions to be approximately uniformly distributed to cover all data regions as good as possible. To achieve this, we use the input parameter $n_{\text{dir\_samp}}$ in the second step of the BROOD sampler. We employ Mitchell's Best-Candidate algorithm to ensure that the sampled points are approximately uniformly distributed on the surface. In every iteration, we sample several potential directions ($n_{\text{dir\_samp}}$) and store the direction with the highest angle between all the previously stored directions. We keep iterating until the number of stored directions equals $n_{\text{dir\_max}}$. A high value of $n_{\text{dir\_samp}}$ will cause the directions to be more uniformly distributed but will slow down computation time. For every ID data point from which we sample, we accordingly scale the directions that we created by sampling on the hypersphere with radius one. [2]

The parameter $\text{dist}_{\text{id\_ood}}$ is used in the BROOD sampler's steps 3 – 6 and captures the distance between the artificial OOD samples and the ID data. This value must have the same meaning over multiple data sets. This prerequisite is met as we use equation (5), exploiting data-dependent scalers, to calculate the distance between two data points.

Further, one can impose that the distance between artificial OOD samples of the same class should be greater than a constant dist_{ood}. Using this, one avoids redundant artificial OOD samples, like duplicates. However, notice that a too high dist_{ood} can cause less adjacent artificial OOD samples.

Finally, when generating artificial OOD samples, we assign the same label to the artificial OOD samples as the ID data point from which they are sampled. In the appendix, we provide an extension of the BROOD sampler that uses the ID data point's neighborhood to assign a label to the artificial OOD samples. This extension did not cause a substantial performance increase in our experiments. Although we assign class-specific labels to the BROOD samples, notice that they do not affect class rations since BROOD samples are inherently different from the actual ID data. Next, our current implementation of the BROOD sampler cannot handle nominal (=categorical) features. We mitigate this problem by encoding nominal features in our data study. An extension of the BROOD sampler that can handle fully categorical or mixed data sets without encoding is a path for future research.

3.2. Out-Of-Distribution Regularized Supervised Machine Learning Models

Let us introduce some additional notation. We denote with v if the data point is artificial ($v = 1$) or not ($v = 0$). We aim to minimize, with $g(\boldsymbol{x}, \boldsymbol{\theta})$ the machine learning's prediction function, the loss

$$L(X, \boldsymbol{y}, \boldsymbol{\theta}) = \frac{1}{n}\Big(\sum_{\boldsymbol{x}: y=1, v=0} l_{00}(g(\boldsymbol{x}, \boldsymbol{\theta})) + \sum_{\boldsymbol{x}: y=0, v=0} l_{10}(g(\boldsymbol{x}, \boldsymbol{\theta})) + \beta_t\Big(\sum_{\boldsymbol{x}: y=0, v=1} l_{01}(g(\boldsymbol{x}, \boldsymbol{\theta})) + \sum_{\boldsymbol{x}: y=1, v=1} l_{11}(g(\boldsymbol{x}, \boldsymbol{\theta}))\Big)\Big). \quad (6)$$

Although the hyper-parameter β_t can be optimized during cross-validation, we always choose $\beta_t = 1$ in our experiments. Further, we make use of the logistic loss that is given by

$$\begin{aligned} l_{00}(g(\boldsymbol{x}, \boldsymbol{\theta})) &= \log\left(1 + \exp\left(g(\boldsymbol{x}, \boldsymbol{\theta})\right)\right) \\ l_{10}(g(\boldsymbol{x}, \boldsymbol{\theta})) &= \log\left(1 + \exp\left(-g(\boldsymbol{x}, \boldsymbol{\theta})\right)\right). \end{aligned} \quad (7)$$

Notice that in the case of a binary response $Y \in (0, 1)$ one finds that

$$\begin{aligned} \text{KL}(P(Y)||P(Y|X)) = P(Y = 1)\log\left(\frac{P(Y = 1)}{P(Y = 1|X)}\right) \\ + (1 - P(Y = 1))\log\left(\frac{1 - P(Y = 1)}{1 - P(Y = 1|X)}\right). \end{aligned} \quad (8)$$

Next, we denote

$$P_{\boldsymbol{\theta}}(Y = 1|X = \boldsymbol{x})) = \frac{1}{1 + \exp\left(-g(\boldsymbol{x}, \boldsymbol{\theta})\right)}. \quad (9)$$

Moreover, let us denote with α the prior of the minority class and with c_{ood_0} and c_{ood_1} constants to scale the prior. These class-dependent different scales enable us to customize the decision surface in data sparse regions. By using equation (8), we determine the loss functions $l_{01}(g(\boldsymbol{x}, \boldsymbol{\theta}))$ and $l_{11}(g(\boldsymbol{x}, \boldsymbol{\theta}))$ that are given by

[2] Define $\tilde{\boldsymbol{v}} = \text{diag}(\hat{h}_1, \ldots, \hat{h}_d) \cdot \boldsymbol{v}$. One can deduce that $\|\boldsymbol{v}\|_{euclid} = \|\tilde{\boldsymbol{v}}\|_{(\text{mahal},\hat{H})}$.

Algorithm 1: Boundary Regularizing Out-Of-distribution (BROOD) Sampler.

Input: X: Covariates, $\mathbf{y}$: Responses, h_{strat}: Captures how to define $\hat{H}$, $\text{query}_{\text{strat}}$: Captures the query strategy, $n_{\text{dir\_max}}$: Maximal number of directions, $n_{\text{dir\_samp}}$: Number of potential directions, $\text{dist}_{\text{id\_ood}}$: The distance between artificial samples and the data point from which they are sampled

Output: X_{brood}: BROOD samples' attributes, y_{brood}: BROOD samples' labels

$\hat{H}_X = \text{scaler}(X, h_{\text{strat}})$ # $\hat{H}_X$ represents scalers for all instances
Denote with d the dimension of X
Determine the ID data points X_{query} (and corresponding $\boldsymbol{y}_{\text{query}}$) we will use to create artificial samples. This strategy is captured in the parameter $\text{query}_{\text{strat}}$

Step 1: Capture data dispersion for every instance in X, using h_{strat}. Determine the ID data points which we will use to create artificial OOD data using $\text{query}_{\text{strat}}$.

$V := \text{dir\_samp}(n_{\text{dir\_samp}}, n_{\text{dir\_max}}, d)$

Step 2: Use $n_{\text{dir\_max}}$ and $n_{\text{dir\_samp}}$ to create and store approximately uniformly distributed directions.

Determine dist_{ood} †
$D_{id} = \text{mahal}(X, X_{\text{query}}, \hat{H}_X)$
$D_{\text{id\_query}} = \text{mahal}(X_{\text{query}}, X_{\text{query}}, \hat{H}_{X_{\text{query}}})$
$\text{NGBH}_{\text{id}} := \text{where}(D_{\text{id}} < 2 \cdot \text{dist}_{\text{id\_ood}}, 1, 0)$ # element wise, 1 if true, else 0
$\text{NGBH2}_{\text{id}} := \text{where}(D_{\text{id\_query}} < 2 \cdot \text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}, 1, 0)$
Keep all data from X that has at least one 1 in NGBH_{id} (in the ID ngbh of X_{query}). We denote with X_{data} the retained data with label $\boldsymbol{y}_{\text{data}}$
$\text{NGBH}_{\text{id\_ood}} = \text{NGBH}_{\text{id}}$

Step 3: To enhance sparseness, define the minimum distance between artificial OOD samples (dist_{ood}). Use $\text{dist}_{\text{id\_ood}}$ and dist_{ood} to determine the relevant neighborhoods of the ID data points from which we will sample. All the ID data points that are not in at least a single neighborhood can be deleted.

for $\boldsymbol{x}_{id}$ *in* X_{query} **do**
  Get label y_{id} of $\boldsymbol{x}_{\text{id}}$
  Use $\text{NGBH}_{\text{id\_ood}}$ to get $X_{\text{NGBH\_id}}$, that is the ID data ngbh of $\boldsymbol{x}_{\text{id}}$ (distance less than $2 \cdot \text{dist}_{\text{id\_ood}}$ and ID data) and corresponding labels $\boldsymbol{y}_{\text{NGBH\_id}}$
  Use $\text{NGBH}_{\text{id\_ood}}$ to get $X_{\text{NGBH\_ood}}$, that is the OOD data ngbh of $\boldsymbol{x}_{\text{id}}$ (distance less than $\text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$ and artificial OOD data) and the corresponding labels $\boldsymbol{y}_{\text{NGBH\_ood}}$
  Use NGBH2_{id} to get $X_{\text{NGBH2\_id}}$, that is the ID data 2 step ngbh of $\boldsymbol{x}_{\text{id}}$ (distance less than $2 \cdot \text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$ and of the same class) and the corresponding labels $\boldsymbol{y}_{\text{NGBH2\_id}}$

Step 4: Query an ID data point from which we will create artificial OOD samples and get the attributes of the data points that are contained in the relevant neighborhoods of the queried ID data point.

  Determine matrix of scaled directions $S_{x_{id}}$ for instance $\boldsymbol{x}_{id}$ using $\text{dir\_scale}(V, \hat{H}_{x_{id}})$
  $X_{\text{samp}} = \boldsymbol{x}_{\text{id}} + S_{x_{id}}$
  $D_{\text{id\_samp}} := \text{mahal}(X_{\text{NGBH\_id}}, X_{\text{samp}}, \hat{H}_{X_{\text{NGBH\_id}}})$
  Use $D_{\text{id\_samp}}$ to determine the minimum distance between each of the samples in X_{samp} and $X_{\text{NGBH\_id}}$
  Delete the samples in X_{samp} with minimum distance from $X_{\text{NGBH\_id}}$ less than $\text{dist}_{\text{id\_ood}}$
  $D_{\text{ood\_samp}} := \text{mahal}(X_{\text{NGBH\_ood}}, X_{\text{samp}}, \min(\hat{H}_{X_{\text{NGBH\_ood}}}, \hat{H}_{x_{id}}))$
  Use $D_{\text{ood\_samp}}$ to determine the minimum distance between each of the samples in X_{samp} and $X_{\text{NGBH\_ood}}$
  Delete the samples in X_{samp} with minimum distance from $X_{\text{NGBH\_ood}}$ less than dist_{ood}
  Create $\boldsymbol{y}_{\text{samp}}$ by assigning the label y_{id} to X_{samp}
  $X_{\text{data}} = X_{\text{data}} \cup X_{\text{samp}}$
  $\boldsymbol{y}_{\text{data}} = \boldsymbol{y}_{\text{data}} \cup \boldsymbol{y}_{\text{samp}}$

Step 5: Investigate the possible directions and keep allowed artificial OOD samples. We delete artificial OOD samples that lie too close to the ID data points and OOD samples of the same label. The artificial OOD samples get the same label as the point from which they are sampled.

  $D_{\text{id2\_samp}} := \text{mahal}(X_{\text{NGBH2\_id}}, X_{\text{samp}}, \hat{H}_{X_{\text{NGBH2\_id}}})$
  Append a column of zeros in $\text{NGBH}_{\text{id\_ood}}$ for every data point in X_{samp}
  Use $D_{\text{id2\_samp}}$ to determine the data points in $X_{\text{NGBH2\_id}}$ which are closer than $\text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$ to at least on instance of X_{samp} and of the same class. Store this information in $\text{NGBH}_{\text{id\_ood}}$

Step 6: If new artificial OOD samples with the same label will be constructed in the future, ensure that the distances toward these new artificial OOD samples will be sufficient.

end
Get X_{brood} by extracting all artificially sampled data points from X_{data}
$\boldsymbol{y}_{\text{brood}}$ equals the artificially sampled data points' labels

† The value of dist_{ood} should be between 0 and the minimum distance between artificial OOD samples generated from the same ID data point. In our experiments, we take dist_{ood} equal to one tenth of the minimum distance between artificial OOD samples generated from the same ID data point.

Algorithm 2: Scaler (scaler(·))

Input: X: Covariates with shape (n, d), h_{strat}: Captures the query strategy
Output: $(H_0, \ldots, H_n)$: vector of scalers
if $h_{strat} = ROT$ **then**
  $\boldsymbol{\sigma} := \text{std}(X)$
  $\hat{\boldsymbol{h}} := \left(\frac{4}{d+2}\right)^{\frac{1}{d+4}} n^{\frac{-1}{d+4}} \boldsymbol{\sigma}$
  Calculate $H_i := \text{diag}\left(1/\hat{\boldsymbol{h}}^2\right)$ for every instance in X # instance independent
end
if $h_{strat} = KNN$ **then**
  Calculate $\boldsymbol{n}_k$ and $\boldsymbol{d}_k$, which respectively equals the k-nearest neighbors and the distance from its k-nearest neighbor from each instance in X
  Calculate $H_i := \text{diag}\left(1/(\sum_{\boldsymbol{x}_i \in n_{j\_k}} d_{i\_k})^2, \ldots, 1/(\sum_{\boldsymbol{x}_i \in n_{j\_k}} d_{i\_k})^2\right)$ for every instance in X # instance dependent
end

Algorithm 3: Direction Sample (dir_samp(·))

Input: $n_{\text{dir\_samp}}$: Number of initial directions, $n_{\text{dir\_max}}$: Maximal number of directions, d: Data dimension
Output: V_{fi} : Matrix of directions
Initialize the matrix of final directions V_{fi} by sampling one sample from a standard normal distribution with d dimensions
while *The number of directions in* V_{fi} *is strictly smaller than* n_{dir_max} **do**
  Obtain a matrix of directions V by sampling $n_{\text{dir\_samp}}$ samples from a standard normal distribution with d dimensions
  Scale the directions accordingly such that their norm equals one
  Construct a matrix of angles Θ between the directions in V_{fi} and V
  Use Θ to find the direction in V with the maximal minimal angle between the directions in V_{fi}. Include this direction in V_{fi}
end

Algorithm 4: Mahalanobis Distance (mahal(·))

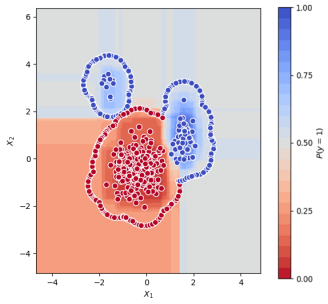
Input: X_a (shape (n_a, d)), X_b (shape (n_b, d)), $(S_0, \ldots, S_{n\_a})$ (components have shape (d, d))
Output: D: Distance matrix (shape (n_a, n_b))
$Z := X_a[:, None, :] - X_b$ (shape (n_a, n_b, d)) # we denote with *None* a dimensional increase
for *Each row i in D* **do**
  $A[i, :] = Z[i, :, :] \cdot S_i$
  $D[i, :] = \sqrt{A[i, :] \cdot Z[i, :, :]^T}$
end

Algorithm 5: Direction Scale (dir_scale(·))

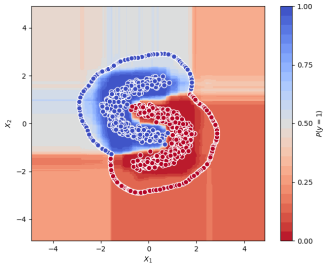
Input: V: Matrix of Directions S: Scaler
Output: V_{sc}: Matrix of scaled directions
$V_s := \sqrt{S^{-1} V}$
$D := \sqrt{V_s S V_s^T}$
$V_{sc} := V_s / D$

$$
\begin{aligned}
l_{01}(g(\boldsymbol{x},\boldsymbol{\theta})) &= c_{ood_0}\alpha \log\left(\frac{c_{ood_0}\alpha}{P_{\boldsymbol{\theta}}(Y=1|X=\boldsymbol{x})}\right) \\
&\quad + (1-c_{ood_0}\alpha)\log\left(\frac{(1-c_{ood_0}\alpha))}{(1-P_{\boldsymbol{\theta}}(Y=1|X=\boldsymbol{x}))}\right) \\
l_{11}(g(\boldsymbol{x},\boldsymbol{\theta})) &= c_{ood_1}\alpha \log\left(\frac{c_{ood_1}\alpha}{P_{\boldsymbol{\theta}}(Y=1|X=\boldsymbol{x})}\right) \\
&\quad + (1-c_{ood_1}\alpha)\log\left(\frac{(1-c_{ood_1}\alpha))}{(1-P_{\boldsymbol{\theta}}(Y=1|X=\boldsymbol{x}))}\right). \quad (10)
\end{aligned}
$$

By using these loss functions, the objective function 6 is convex. We impose that $c_{ood_1}\alpha$ and $c_{ood_0}\alpha$ are bounded by 0 and 1. Further, notice that at these bounds, the loss functions (10) are the same as the logistic loss functions (7). In figure 2, we again visualize our toy data sets with the decision surfaces trained with XGBoost. Now, we also include the artificially generated OOD samples that we used to train the decision surfaces. One can indeed deduce that the OOD samples can regularize the decision surface and that the class-dependent constants can emphasize certain data regions.



Visual of the toy data set with BROOD samples.



Visual of the moons data set with BROOD samples.

Figure 2: Visual of decision surfaces and generated BROOD samples. The XGBoost classifier is trained using a regularizing loss. For the toy data set, we use $c_{ood_1} = 2$ and $c_{ood_0} = 1$. For the moons data set, we set $c_{ood_1} = 1$ and $c_{ood_0} = 0.2$.

3.3. The Effect Of The BROOD Sampler's Hyper-parameters

Before we investigate our methodology in a real-life setting, we discuss the effect of the BROOD sampler's hyper-parameters on both the generation of BROOD samples and the training of decision surfaces.

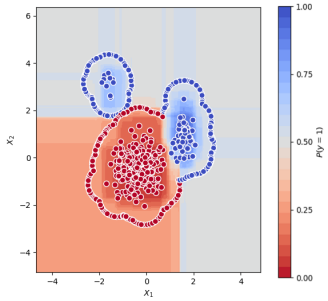
First, let us discuss $n_{\text{dir\_samp}}$ and $\text{query}_{\text{strat}}$. As previously mentioned, a high value of $n_{\text{dir\_samp}}$ will cause the directions to be more uniformly distributed. Concerning $\text{query}_{\text{strat}}$, we regularise the OOD spaces close to the instances from which we sample. For example, sampling from minority instances results in regularized OOD spaces close to the minority instances. We denote $\text{query}_{\text{strat}}$ = ALL if we sample from all instances and we denote $\text{query}_{\text{strat}}$ = MIN if we sample from the minority instances.

The parameter h_{strat} determines how we grasp the dispersion of the data. In subsection 3.1, we proposed multiple ways to achieve this goal. From now, we denote h_{strat} = ROT if we use equation 2 to grasp data dispersion. The rule of thumb selector differs in every dimension and is the same for every instance. Hence, we actually create directions on a multidimensional instance-independent ellipse. Next, we denote h_{strat} = KNN if we use equation 3 to grasp data dispersion. In this case, $\hat{\boldsymbol{h}}$ is constant but instance-dependent. Hence, we create directions on a multidimensional sphere with an instance-dependent radius. The top images of figure 3 visualize the effect of this hyper-parameter.

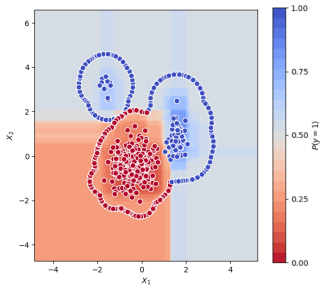
The parameter $\text{dist}_{\text{id\_ood}}$ determines the distance from the ID data points to the BROOD samples. A too low $\text{dist}_{\text{id\_ood}}$ will cause the BROOD samples to interfere with the ID data (i.e. introduce noise) and will negatively influence computation time due to the construction of an excessive number of BROOD samples. However, a too high $\text{dist}_{\text{id\_ood}}$ will attenuate the regularizing effect of the BROOD samples. As the distance of the BROOD samples from the ID data increases, the distance between the BROOD samples will also increase, and more BROOD samples will be needed to fully regularize the decision surface. Further, if the BROOD samples are too far away from the ID data points, the decision surface will be more chaotic between the ID data and BROOD samples. The images in the middle of figure 3 visualize the effect of $\text{dist}_{\text{id\_ood}}$ on the generation of BROOD samples and the decision surface trained by XGBoost in these extreme cases.

Next, the parameter $n_{\text{dir\_max}}$ determines the maximum number of artificial samples created from one ID sample. Thus, on the one hand, a too low $n_{\text{dir\_max}}$ will not provide sufficient BROOD samples to fully regularize the decision surface. On the other hand, a too high $n_{\text{dir\_max}}$ will have a negative influence on computation time due to an excessive number of training points. Additionally, without a proper weighting strategy, a too high $n_{\text{dir\_max}}$ diminishes the importance of the existing ID data points. One can find visualizations on the bottom side of figure 3.

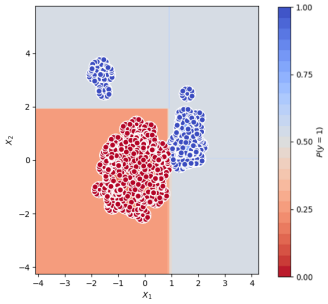
Notice that the number of dimensions can affect the optimal value of the $n_{\text{dir\_max}}$ parameter. Like other existing oversampling techniques, our method suffers from the curse of dimensionality as it is more challenging to cover multi-dimensional data regions with only a few data points. Hence, for high-dimensional problems, an optimal OOD sampling strategy will generally require more OOD samples and thus require more computational effort.



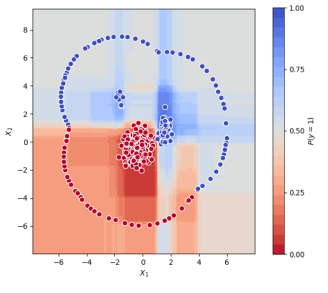
Visual of BROOD samples with h_{strat} = ROT, $\text{dist}_{\text{id\_ood}} = 2$, and $n_{\text{dir\_max}} = 50$.



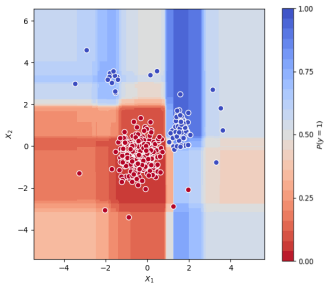
Visual of BROOD samples with h_{strat} = KNN, $\text{dist}_{\text{id\_ood}} = 0.75$, and $n_{\text{dir\_max}} = 50$.



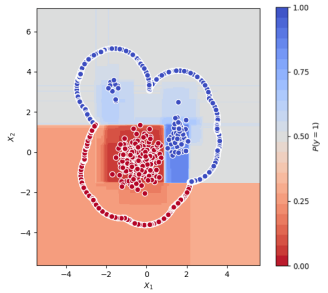
Visual of BROOD samples with a low $\text{dist}_{\text{id\_ood}}$ value. We take h_{strat} = ROT, $\text{dist}_{\text{id\_ood}} = 0.5$, $n_{\text{dir\_max}} = 50$.



Visual of BROOD samples with a high $\text{dist}_{\text{id\_ood}}$ value. We take h_{strat} = ROT, $\text{dist}_{\text{id\_ood}} = 10$, and $n_{\text{dir\_max}} = 50$.



Visual of BROOD samples with a low $n_{\text{dir\_max}}$ value. We take h_{strat} = ROT, $\text{dist}_{\text{id\_ood}} = 4$, and $n_{\text{dir\_max}} = 5$.



Visual of BROOD samples with a high $n_{\text{dir\_max}}$ value. We take h_{strat} = ROT, $\text{dist}_{\text{id\_ood}} = 4$, $n_{\text{dir\_max}} = 500$.

Figure 3: Visual comparison of the effect of the BROOD sampler's hyper-parameters. We visualise the effect of h_{strat}, $n_{\text{dir\_max}}$, and $\text{dist}_{\text{id\_ood}}$ on the generation of BROOD samples and the decision surface trained on a toy data set. We always take $\text{query}_{\text{strat}}$ = ALL and $n_{\text{dir\_samp}} = 90$. We impose that $c_{ood_1} = 2$ and $c_{ood_0} = 1$ and keep all XGBoost's hyper-parameters constant.

Hence, one should optimize these hyper-parameters using the validation set to achieve optimal performance, which can be pretty time-consuming. Thus, there is a serious need to propose some initial rules or best practices.

Using h_{strat} = ROT, the bandwidth actually represents the standard deviation parameter of the Gaussian kernel. It is a well-known heuristic that, for a Gaussian distribution, almost all data points have a distance less than three times the standard deviation from the mean. Hence, in this case, we reason that $\text{dist}_{\text{id\_ood}}$ should be greater than three in most cases. Further, as discussed before, $\text{dist}_{\text{id\_ood}}$ should not be too large as this has several negative implications. From our analysis, we noticed that $\text{dist}_{\text{id\_ood}}$ should be smaller than seven. As the rule of thumb estimator accounts for the number of dimensions, we believe the effect of the number of dimensions on this parameter is minimal. We found that one achieves good results on many data sets by taking $\text{dist}_{\text{id\_ood}} = 4$ if h_{strat} = ROT.

Next, we derive a similar rule if one takes h_{strat} = KNN. Denote with S_d^r the surface area of a d-dimensional hyper-sphere with radius r. The k-nearest neighbor density estimator proposed in [29] equals

$$\hat{P}(\boldsymbol{x}_j) = \frac{k}{nS_d^1(d_{j_k})^d} \tag{11}$$

for $\boldsymbol{x}_j$. Hence, only the k instances with a distance smaller or equal to $d_{j,k}$ contribute to this nearest neighbor estimate. Hence, following this reasoning, $\text{dist}_{\text{id\_ood}}$ should be greater than one. Further, from our experiments, we recommend that $\text{dist}_{\text{id\_ood}}$ should be smaller 2. We obtain good results on many data sets by taking $\text{dist}_{\text{id\_ood}} = 1.5$. In [29], one reasons that the optimal $k = O\left(n^{4/(d+4)}\right)$. By taking $k = 2n^{4/(d+4)}$, we are able to achieve satisfactory performance.

In our experiments, we always take $n_{\text{dir\_max}} = 30$ and $n_{\text{dir\_samp}} = 90$.

4. Experiments

In the next section, we perform an extensive data study to evaluate the performance of our proposed machine learning models. First, we discuss the balanced and imbalanced classification data sets we will use in our experiments. Further, we elaborate on our experimental methodology and introduce various performance metrics. Finally, we discuss whether BROOD samples are able to enhance the machine learning model's performance and deduce whether our approach complements existing oversampling techniques.

4.1. Experimental Design

4.1.1. Data Sets

First, we compare BROOD-enhanced models with their standard counterparts on 15 real-world benchmark data sets for binary classification. We test our models on the UCI [dataset][13] ecoli, mammographic masses, sonar, ionosphere, breast cancer Wisconsin, heart, Indian liver patient, liver disorders, breast cancer, vehicle, contraceptive method, German credit card, credit approval, bank marketing, and madelon data set. All these data sets, and corresponding code, can be found on GitHub[3]. The term 'benchmark data sets' encapsulates all the previous data sets for conciseness. One can find the benchmark data sets' summary in table 1. The data sets can consist of numerical (N) and categorical (C) features.

Next, we test our BROOD-enhanced machine learning models on multiple difficult to train imbalanced data sets. We test our models on data from the ESA Polish Bankruptcy data set [dataset][13], financial distress data set [dataset][14], UCI German credit card, UCI credit approval and UCI bank marketing data set [dataset][13], IBM Telco Customer Churn data set [dataset][5], ETL Credit Card Approval data set [dataset][30], VUB credit scoring data set [dataset][54], KDD Cup 1998 data

[3] https://github.com/CFLDT/Regularization-Oversampling-for-Classification-Tasks-To-Exploit-What-You-Do-Not-Know

	Class 1	Class 0	# Samples	Ratio	# Dimensions
UCI Ecoli (N)	pp	all other	366	0.155	7
UCI Mammographic Masses (C)	1	0	961	0.463	4
UCI Sonar (N)	M	R	208	0.536	60
UCI Ionosphere (N)	b	g	351	0.359	34
UCI Breast Cancer Wisconsin (N)	M	B	569	0.373	30
UCI Heart (N & C)	2	1	270	0.444	13
UCI Indian Liver Patient (N & C)	2	1	583	0.286	10
UCI Liver Disorders (N)	consumption > 0.5	consumption ≤ 0.5	345	0.339	5
UCI Breast Cancer (C)	recurrence -events	no-recurrence -events	286	0.297	9
UCI Vehicle (N)	VAN	all others	964	0.235	18
UCI Contraceptive method (C)	long term	all others	1,473	0.226	9
UCI German Credit Card (N & C)	2	1	1,000	0.300	20
UCI Credit Approval (N & C)	+	−	690	0.445	15
UCI bank Marketing (N & C)	yes	no	4,119	0.109	20
UCI Madelon (N)	1	0	2,600	0.500	501

Table 1: Summary of the benchmark data sets. The data sets can consist of numerical (N) and categorical (C) features.

set [dataset][37], (private) car insurance fraud data set, (private) APATE credit card fraud data set, JAR financial statement fraud data set [dataset][58], IEEE-CIS customer transaction fraud data set [dataset][48], synthetic mobile transaction fraud data set [dataset][41], and synthetic credit card fraud data set [dataset][15]. The ESA Polish Bankruptcy data set contains financial rates from a forecasting period of a year and bankruptcy status after five years of Polish companies. The data set consists of operating companies between 2000 and 2012 and bankrupt companies between 2007 and 2013 [62]. The financial distress data set involves information concerning the financial distress for a sample of companies. The UCI German credit card data set classifies people as good or bad credit risks and the UCI Credit Approval data contains credit card applications[13]. The UCI bank marketing data set contains information from a direct marketing campaign from May 2008 to November 2010 of a Portuguese banking institution [34]. The IBM Telco Customer Churn contains data from a fictional telco company's customers and their churn behaviour. The ETL Credit Card Approval data set involves information concerning credit card applicants. The VUB credit scoring data set consists of accepted loans given to individual customers from January 2016 to December 2016 by a Romanian NBFI [38]. The KDD data set contains information on a direct mailing campaign and donations and has been used for the second international knowledge discovery and data mining tools competition. Next, we received the private car insurance fraud data set from an international insurer. The data set consists of a sample of fraudulent and non-fraudulent Belgian auto-mobile claims from 2012 until 2021. The APATE credit card fraud data set consists of fraudulent and non-fraudulent transactions from a large Belgian credit card issuer [51]. We use an already pre-processed version of this data set in our study. The JAR financial statement fraud data set is a manually gathered data set [4] that contains accounting fraud samples from the SEC's Accounting and Auditing Enforcement Releases (AAERs), enhanced with financial accounting data. The data set consists of fraud and legitimate instances between 1990 and 2014. The IEEE-CIS customer transaction fraud data set consists of real-world e-commerce transactions. The synthetic mobile transaction fraud data set is a synthetic data set based on a sample of real transactions from a mobile money service in an African country over multiple periods. Finally, the synthetic credit card fraud data set is a synthetic data set that contains transactions of synthetic consumers who reside in the United States.

We execute some additional pre-processing steps for some imbalanced data sets. We randomly under-sample certain imbalanced data sets to ensure empirical tractability. Further, if the data set is not severely imbalanced, we randomly under-sample its minority class. We use the provided summary variables for the KDD data set to include the promotion and donation histories. The JAR financial statement fraud data set spans several periods [4]. The fact that the train and test set could contain the same firm (and that the data contains firm-specific characteristics) can seriously enhance the performance of the machine learning methods [55]. To ensure that no serial cor-

relation is present in the financial statement fraud data set, we only keep the first fraud case of a particular firm in the data set. For the synthetic mobile transaction fraud data set, we extract the first 8 periods of the simulation. Next, we create aggregated features that, for instance, capture the number of transactions the recipient already received during this period. For the synthetic credit card fraud data set, we extract the first 3 customers of the simulation. For this data set, we also create aggregate features that, for instance, capture the number of transactions the customer has done in the last 24 hours. One can find a summary of the imbalanced data sets after these general pre-processing steps in table 2. Despite the private car insurance fraud data set and private APATE credit card fraud data set, one can find all pre-processed imbalanced data sets used in this paper on GitHub.

4.1.2. Methodology

We use random stratified sampling to obtain an initial train set consisting of 75% of all instances and a test set consisting of 25% of all instances. Furthermore, we split the initial train set (in a stratified way) into the final train set (50% of all instances) and a validation set (25% of all instances). We train the model on the final train set, use the validation set to optimize the models' hyper-parameters, and assess performance on the test set. We execute this procedure four times in a row for every data set, each time with a completely different test set.

We train logistic regression benchmark models and XGBoost [9] models with and without artificially generated BROOD samples. Logistic regression is the typical benchmark model and is widely used in various experimental studies. The XGBoost algorithm is a boosted tree algorithm that involves combining many trees and uses gradient information to choose the direction it needs to improve the fit to the data. The XGBoost algorithm is known to be computationally efficient and can control for over-fitting. One can find more details about our pipeline and the set of hyper-parameters in the appendix.

We use three evaluation metrics to assess the performance of our algorithms. First, we compare the Area Under the Receiving Operating Curve (ROC-AUC) of the different models to compare the aggregate performance (over different thresholds) and minimize misclassification errors [47]. In short, the ROC-AUC measures how well a model can distinguish the two classes. We denote with $\text{TPR}(\phi) = \mathbb{E}_{y_1}[g_\phi(\boldsymbol{x}, \boldsymbol{\theta})]$ the true positive rate for threshold ϕ and with $\text{FPR}(\phi) = \mathbb{E}_{y_0}[g_\phi(\boldsymbol{x}, \boldsymbol{\theta})]$ the false positive rate for threshold ϕ. The ROC-AUC is equal to

$$\text{ROC-AUC} = \int_0^1 \text{TPR}(\phi) d\text{FPR}(\phi). \tag{12}$$

Next, we compare the average precision (AP). The AP equals the sum of precisions, with the increase in TPR (also known as recall) over different thresholds as weights. This measure is suitable for imbalanced learning as it does not incorporate the algorithm's ability to detect majority instances. The precision equals $\text{PR}(\phi) = \mathbb{E}_{y_1}[g_\phi(\boldsymbol{x}, \boldsymbol{\theta})]/\mathbb{E}_y[g_\phi(\boldsymbol{x}, \boldsymbol{\theta})]$ for threshold ϕ. Over thresholds $\phi_1, \ldots, \phi_n$, the AP equals

$$\text{AP} = \sum_{i \in (2,\ldots,n)} \Big(\text{TPR}(\phi_i) - \text{TPR}(\phi_{i-1})\Big)\text{PR}(\phi_i). \tag{13}$$

Finally, we use the Discounted Cumulative Gain (DCG) that was also used in [4] to assess financial statement fraud. This metric is material for fraud detection algorithms as there often are insufficient resources to investigate all the suspicious cases. Similarly, in churn and marketing data sets, there is only limited budget to target certain customers. Hence, detecting fraud, and targeting valuable customers can be seen as a ranking problem. The formula of discounted cumulative gain that we use in our analysis is given by

$$\text{DCG}(b) = \sum_{i=1}^{b} \frac{2^{\text{rel}_i} - 1}{\log_2(i+1)}. \tag{14}$$

The relevance (rel) equals one if the instance is part of the positive class and zero otherwise. We can limit the performance evaluation to only a small number (i.e., b as defined above) of data points with the highest predicted probability. We take the parameter b equal to the number of instances in the positive class in the test set.

To compare all classifiers to each other, we use the non-parametric Nemenyi test and construct critical difference plots [10]. The Nemenyi test for pairwise comparisons of k classifiers on n data sets with critical value q_α (confidence level α) states that if their rank differs by at least the critical difference (CD)

$$\text{CD} = q_\alpha \sqrt{\frac{k(k+1)}{6n}}, \tag{15}$$

the classifiers are significantly different. In the figures that we construct, the classifiers connected by the bold horizontal line represent the not significantly different classifiers with a confidence level of 0.90.

Let us discuss the BROOD sampler's hyper-parameters used in our experiments and introduce some new notations to enhance conciseness. First, we always take $n_{\text{dir\_max}} = 30$ and $n_{\text{dir\_samp}} = 90$. We denote with 'ALL' if $\text{query}_{\text{strat}} = \text{ALL}$ and we denote with 'MIN' if $\text{query}_{\text{strat}} = \text{MIN}$. We use the notation 'ROT' if we generate BROOD samples by taking $h_{\text{strat}} = \text{ROT}$ and $\text{dist}_{\text{id\_ood}} = 4$. Furthermore, We use the notation 'KNN' if we generate BROOD samples by taking $h_{\text{strat}} = \text{KNN}$ and $\text{dist}_{\text{id\_ood}} = 1.5$. For example, BROOD(ALL_ROT) uses all instances to generate OOD samples with $n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $h_{\text{strat}} = \text{ROT}$, and $\text{dist}_{\text{id\_ood}} = 4$. We never optimize the BROOD sampler's hyper-parameters to substantiate its real-life practicability. We do not claim that any of our proposed hyper-parameter combinations are optimal.

Next, we impose that β_t (see equation 6) equals one[4]. Finally, we find that logistic regression models are not able to

[4]Nevertheless, to obtain the best performance, one should tune β_t. If the inclusion of artificial samples (SMOTE, ADASYN, ROSE, BROOD, ...) reduces the model's performance on the validation set, it would not be very smart to use them for training the model. Second, if the number of BROOD samples

	Class 1	Class 0	# Samples	Ratio	# Dimensions
ESA Polish Bankruptcy (N)	1	0	7,027	0.0386	64
Financial Distress (N)	financial distress < -0.5	financial distress ≥ -0.5	3,672	0.0370	84
UCI German Credit Card IMB (N & C)	2	1	760	0.0789	20
UCI Credit Approval IMB (N & C)	+	-	414	0.0749	15
UCI Bank Marketing IMB (N & C)	yes	no	3,758	0.0239	20
IBM Telco Customer Churn (N & C)	Yes	No	5,548	0.0674	19
ETL Credit Card Approval (N & C)	1	0	12,654	0.0043	17
VUB Credit Scoring (N & C)	1	0	16,352	0.0392	18
KDD Cup 1998 (N & C)	1	0	14,312	0.0519	394
(Private) Car Insurance Fraud (N & C)	1	0	16,308	0.0210	23
(Private) APATA Credit Card Fraud (N & C)	True	False	7,279	0.0076	7
JAR Financial Statement Fraud (N & C)	1	0	14,910	0.0270	42
IEEE-CIS Customer Transaction Fraud (N & C)	1	0	11,811	0.0328	391
Synthetic Mobile Transaction Fraud (N & C)	1	0	3,591	0.0251	13
Synthetic Credit Card Fraud (N & C)	Yes	No	5,784	0.0214	15

Table 2: Summary of the severely imbalanced data sets. The data sets can consist of numerical (N) and categorical (C) features. To ensure severe imbalance and analytical tractability, certain data sets are undersampled versions of the original data sets.

handle the non-linearities that can arise from the BROOD samples in particular data sets. Hence, we decide not to discuss BROOD-enhanced logistic regression models.

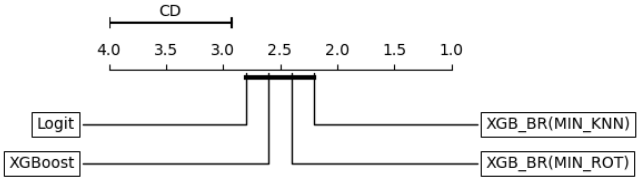
4.2. Experimental Results

4.2.1. Benchmark Data Sets

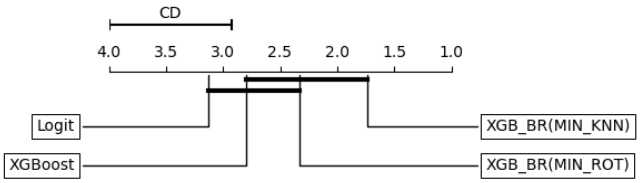
We impose a maximum of 10,000 BROOD samples on the benchmark data sets. If this bound is reached, we only create BROOD samples from the most outlying data points. We create critical difference diagrams to assess the difference in the predictive power of the machine learning models with a significance level of 0.10. We always include logistic regression as a benchmark model.

Figure 4 visualizes the Nemenyi test on ROC-AUC, AP and DCG of the different classifiers on the benchmark data sets. First, we find that the XGBoost model outperforms the logistic regression model for all the performance metrics (although not significant). This can be explained by the fact that XGBoost can construct non-linear decision boundaries. Next, due to the simplicity of the benchmark data sets, there are likely none (or a limited number) of OOD data points in the test sets. Hence, it is essential to show that the possibility of using BROOD samples does not result in over-fitting or a performance decrease (or both) on the test set. For the ROC-AUC, on which we cross-validate, we can deduce that the normal and BROOD-enhanced XGBoost achieve similar performance.Although we did optimize the model's hyper-parameters on the ROC-AUC, the other performance metrics shed some light on the power of BROOD samples. We also find that the BROOD-enhanced XGBoost models ~~substantially perform better~~ in general perform at least as well as the regular XGBoost model on the AP and DCG metrics. Furthermore, the BROOD(ALL_KNN)-enhanced XGBoost classifier performs better than the BROOD(ALL_ROT)-enhanced XGBoost classifier on all performance metrics on the benchmark data sets. Table 3 contains the average number of artificial BROOD samples created during training. On average, the
BROOD(ALL_KNN) sampler samples fewer artificial points than the BROOD(ALL_ROT) sampler.

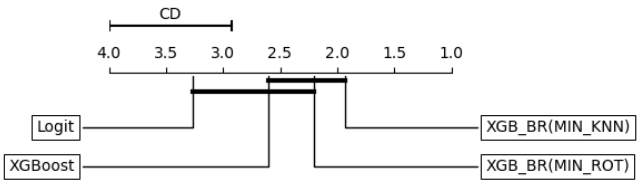
is low or high compared to the number of ID samples, it may be appropriate to weigh them appropriately. Finally, one can interpret the terms that account for BROOD samples in the objective function as regularization terms, and one often optimizes the weight of such terms.



Critical difference diagram of the benchmark data sets by using the ROC-AUC metric.



Critical difference diagram of the benchmark data sets by using the AP metric.



Critical difference diagram of the benchmark data sets by using the DCG metric.

Figure 4: Performance metrics: critical difference diagrams with significance level 0.10 of the models trained on the benchmark data sets. We use BROOD(ALL_ROT) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 4$) and BROOD(ALL_KNN) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 1.5$) to generate BROOD samples. We abbreviate 'XGBoost' as ' XGB' and 'BROOD' as 'BR'.

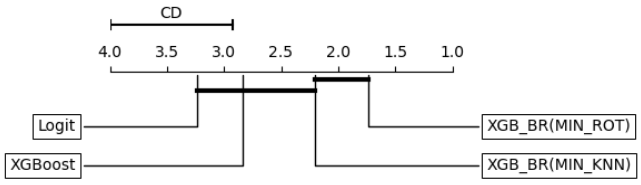
4.2.2. Severely Imbalanced Data Sets

This section examines the usefulness of the BROOD sampler for developing machine learning models on severely imbalanced data sets that are difficult to train. We investigate if BROOD samples can aid machine learning models in learning a suitable decision surface to classify positive instances correctly.

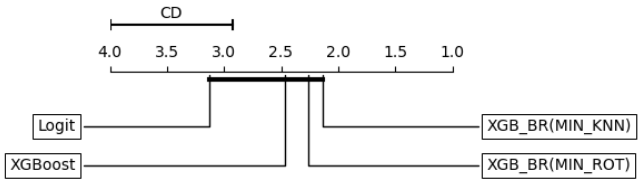
Hence, both AP and DCG are suitable metrics as one is more interested in the model's ability to detect minority instances in many applications. Furthermore, in many applications, one only has a limited pool of resources to target positive instances. In this case, the DCG is even more appropriate as it is only affected by the most likely positive instances in the test set. Hence, we use the DCG to optimize the model's hyper-parameters during cross-validation in this subsection.

The query strategies' decision (this captures the ID data points from which we will sample) is related to the previous paragraph. We are less interested in the model's ability to classify majority instances correctly. Hence, we decide to sample BROOD samples from the minority class to indicate the OOD spaces closer to the minority instances. Furthermore, this allows us to compare BROOD sampling with existing minority oversampling techniques. As the number of positive instances is limited, the BROOD sampler will be quite fast, and the number of BROOD samples will be relatively low. This implies that the negative impact of sampling on the computation time is limited.

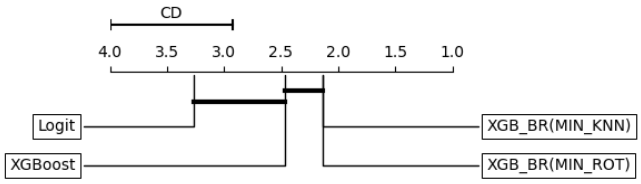
In general, by creating BROOD samples on a limited number of data points (only the minority instances), we find that the BROOD-enhanced XGBoost models perform at least as well as the regular XGBoost model on the severely imbalanced data sets. Moreover, we find that the XGBoost models that exploit BROOD samples using the rule of thumb selector with the standard hyper-parameters seriously outperform the regular counterpart on the DCG metric on these data sets. ~~as we find a considerable difference between the regular and BROOD-enhanced XGBoost classifiers for the DCG metric. Hence, by creating BROOD samples on a limited number of data points (only the minority instances), one can notably improve this material performance metric in imbalanced classification.~~ Moreover, we find that the BROOD-enhanced XGBoost classifiers ~~slightly outperform~~ are at least able to attain a similar performance as the standard XGBoost model on the ROC-AUC and AP. The BROOD(MIN_ROT)-enhanced XGBoost classifier performs better than the BROOD(MIN_KNN)-enhanced XGBoost classifier on these data sets. One can find the numerical values of the various performance metrics in table 10 in the appendix.



Critical difference diagram of the severely imbalanced data sets by using the DCG metric.



Critical difference diagram of the severely imbalanced data set by using the AP metric.



Critical difference diagram of the severely imbalanced data sets by using the ROC-AUC metric.

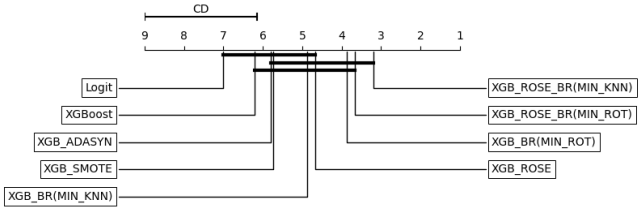
Figure 5: Performance metrics: critical difference diagrams with significance level 0.10 of the models trained on the severely imbalanced data sets. We use BROOD(MIN_ROT) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 4$) and BROOD(MIN_KNN) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 1.5$) to generate BROOD samples. The best-performing model is in bold. We abbreviate 'XGBoost' as ' XGB' and 'BROOD' as 'BR'.

Remember that existing minority oversampling techniques aim to cover more broad data regions to aid the machine learning models in learning less specific data regions. Our oversampling technique aids in regularizing the machine learning model's decision surface by assigning pre-determined probabilities in previously unseen data regions. Although the purpose

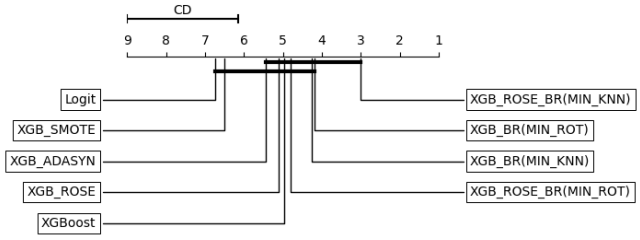
of BROOD sampling is different, it is interesting to assess the performance differences on the severely imbalanced data sets.

We find that ROSE is the best-performing minority oversampling technique. We include the combination of both ROSE and BROOD sampling to investigate whether BROOD samples complement existing minority oversampling methods. We first execute the ROSE sampler on the train set and execute the BROOD sampler on real minority data points and synthetic ROSE minority samples with the previously mentioned hyperparameters.

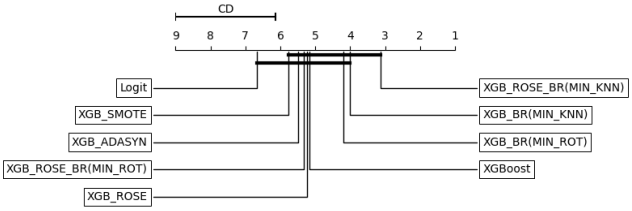
The performance of all our models on the imbalanced data sets can be found in figure 6. In general, we find that BROOD samples are able to ~~improve~~ enhance classifier performance on all performance metrics on the imbalanced data sets. Next, we see that all XGBoost models that exploit artificial samples ~~outperform~~ perform at least as well as the standard XGBoost model on the DCG metric, on which we cross-validate. Moreover, we find that the XGBoost models exploiting both ROSE and BROOD samplers outperform all models on the DCG metric on the imbalanced data sets. Even stronger, the DCG of the XGBoost model exploiting both ROSE and BROOD(MIN_KNN) samples is significantly different compared to the standard XGBoost model. One can find the numerical values of the various performance metrics in table 10 in the appendix. Next, table 4 contains the average number of artificial BROOD samples created during training.



Critical difference diagram of the severely imbalanced data sets by using the DCG metric.



Critical difference diagram of the severely imbalanced data sets by using the AP metric.



Critical difference diagram of the severely imbalanced data sets by using the ROC-AUC metric.

Figure 6: Performance metrics: critical difference diagrams with significance level 0.10 of the models trained on the severely imbalanced data sets. We use BROOD(MIN_ROT) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 4$) and BROOD(MIN_KNN) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 1.5$) to generate BROOD samples. We use the imbalance ratio that on average performs best on all data sets. The stand alone SMOTE, ADASYN, and ROSE samplers aim to achieve an imbalance ratio of 0.20. The ROSE sampler along with the BROOD sampler aim to achieve an imbalance ratio of 0.10. The best-performing model is in bold. We abbreviate 'XGBoost' as ' XGB' and 'BROOD' as 'BR'.

5. Discussion

We wrote this manuscript to address the arbitrary overconfidence of discriminative machine learning methods in unseen data regions. We believe that this issue has not yet received enough attention, and many methodologies tackling this problem can still be explored. We mitigate this problem by sampling artificial points on the edge of the training data using the BROOD sampler.

On the other hand, minority oversampling methods for imbalanced classification are very popular and well-documented. Imbalanced classification is also an application where BROOD samples can improve performance. Of course, discriminative machine learning models tend to be overconfident in unseen data regions, and imbalanced data sets lack sufficient information to model the minority class correctly. As the goal of minority oversampling and OOD sampling is inherently different, their combination has not been discussed in previous literature. By writing this manuscript, we also aim to inspire researchers

to investigate new usages of artificial samples in machine learning.

Of course, our methodology and research have several limitations. First, BROOD samples have little value in applications where one does not encounter data points in unseen data spaces during the test/production phase. Next, like all oversampling methods, our method increases learning time. Furthermore, BROOD samples can diminish the importance of the original data points and improperly generated BROOD samples can add little value or even introduce noise. As discussed before, our current implementation of the BROOD sampler cannot handle nominal (=categorical) features.

We did compare our model in an extensive data study with benchmark models and existing popular minority oversamplers. However, comparisons with existing OOD samplers result in some incompatibility issues. Existing research generally uses GANs or VAEs, which are often too complex for tabular and low-dimensional data. Moreover, existing OOD samplers usually do not distinguish between class labels, which gives comparability issues for the imbalanced data set experiment, where we only sample from minority instances. Furthermore, OOD samples are often used for other goals like OOD detection or open-set recognition. This is inherently different from our goal in the experiments, which is to improve classifier performance (without any unseen classes). Finally, existing OOD samplers differ in choosing/bounding the number of OOD samples, which is an important parameter and can seriously affect classifier performance. A survey paper discussing and comparing existing OOD oversamplers in different fields and applications is an exciting path for further research.

	ALL_ROT		ALL_KNN	
UCI Ecoli	440.00	(1) 61.00 (0) 379.00	368.00	(1) 43.25 (0) 324.75
UCI Mammographic Masses	153.25	(1) 101.25 (0) 52.00	169.25	(1) 101.25 (0) 68.00
UCI Sonar	3,059.50	(1) 1,660.75 (0) 1,398.75	1,470.75	(1) 803.00 (0) 667.75
UCI Ionosphere	3,772.25	(1) 1,806.25 (0) 1,966.00	3,118.00	(1) 1,585.50 (0) 1,532.50
UCI Breast Cancer Wisconsin	7,501.00	(1) 3,055.25 (0) 4,446.25	4,603.50	(1) 1,966.50 (0) 2,637.00
UCI Heart	2,372.75	(1) 1,140.00 (0) 1,232.75	940.75	(1) 464.00 (0) 476.75
UCI Indian Liver Patient	1,614.50	(1) 203.00 (0) 1,411.5	1,001.75	(1) 212.50 (0) 789.25
UCI Liver Disorders	559.75	(1) 159.00 (0) 400.75	397.75	(1) 137.25 (0) 260.50
UCI Breast Cancer	958.25	(1) 386.00 (0) 572.25	401.75	(1) 168.50 (0) 233.25
UCI Vehicle	5,483.50	(1) 1,241.50 (0) 4,242.00	2,341.25	(1) 571.25 (0) 1,770.00
UCI Contraceptive method	1,473.75	(1) 200.75 (0) 1,273.00	576.00	(1) 105.25 (0) 470.75
UCI German Credit Card	4,583.00	(1) 1,632.25 (0) 2,950.75	1,256.00	(1) 458.75 (0) 797.25
UCI Credit Approval	3,909.75	(1) 2,079.50 (0) 1,830.25	1,897.50	(1) 1,047.75 (0) 849.75
UCI Bank Marketing	9,724.25	(1) 3,391.50 (0) 6,332.75	4,298.25	(1) 1,116.00 (0) 3,183.75
UCI Madelon	9,985.75	(1) 4,436.00 (0) 5,549.75	9,994.75	(1) 4,726.75 (0) 5,268.00

Table 3: The average number of BROOD samples for the benchmark data sets. We use BROOD(ALL_ROT) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 4$) and BROOD(ALL_KNN) ($n_{\text{dir\_max}} = 30$, $n_{\text{dir\_samp}} = 90$, $\text{dist}_{\text{id\_ood}} = 1.5$) to generate BROOD samples. We impose a maximum bound of $10,000$ BROOD samples. The sum of the average number of BROOD samples sampled from class 1 (denoted with (1)) and class 0 (denoted with (0)) equals the total number of average BROOD samples.

	MIN_ROT	MIN_KNN	ROSE_MIN_ROT	ROSE_MIN_KNN
ESA Polish Bankruptcy	404.75	404.25	5,980.00	729.25
Financial Distress	1,504.00	84.50	4,645.25	496.25
UCI German Credit Card IMB	558.50	165.50	655.75	191.50
UCI Credit Approval IMB	379.75	206.50	474.50	218.00
UCI Bank Marketing IMB	954.75	370.00	4,740.50	1,657.00
IBM Telco Customer Churn	2,961.50	1,161.75	4,360.00	1,836.25
ETL Credit Card Approval	242.75	71.75	6,649.00	831.75
VUB Credit Scoring	2,521.75	925.50	10,990.00	5,319.75
KDD Cup 1998	9,128.25	2,323.50	17,257.50	3,957.75
(Priv.) Car Insurance Fraud	2,372.75	977.50	19,713.75	6,476.25
(Priv.) APATA Credit Card Fraud	425.00	50.00	1,564.25	558.00
JAR Financial Statement Fraud	2,003.50	1,580.50	17,424.75	13,338.00
IEEE-CIS Cus. Trans. Fraud	2,728.50	142.00	13,944.00	267.00
Synth. Mobile Trans. Fraud	159.50	136.25	1,444.75	528.25
Synthetic Credit Card Fraud	1,623.50	466.75	7,428.75	1,711.75

Table 4: The average number of BROOD samples for the severely imbalanced data sets. We use BROOD(MIN_ROT) ($n_{\text{dir\_max}}$ = 30, $n_{\text{dir\_samp}}$ = 90, $\text{dist}_{\text{id\_ood}}$ = 4) and BROOD(MIN_KNN) ($n_{\text{dir\_max}}$ = 30, $n_{\text{dir\_samp}}$ = 90, $\text{dist}_{\text{id\_ood}}$ = 1.5) to generate BROOD samples. We use the imbalance ratio that on average performs best on all data sets. The ROSE sampler along with the BROOD sampler aim to achieve an imbalance ratio of 0.10.

6. Conclusion And Future Research

In this paper, we develop a methodology that mitigates the excessive confidence of discriminative machine learning models in regions where little information is known. We propose the easily customizable BROOD sampler that generates artificial data points at the boundary of the training data.

This sampler allows assigning a customized probability to OOD regions, ~~solving~~ mitigating the unfounded randomness and overconfidence of discriminative classifiers in unseen data regions. ~~Due to this flexibility, we can enhance machine learning models' performance on benchmark and severely imbalanced data sets. We found that the BROOD-enhanced XGBoost models are able to seriously outperform their standard counterparts on material performance metrics for imbalanced classification.~~ We show that the BROOD-enhanced XGBoost models perform at least as well as the regular XGBoost model on balanced and imbalanced data sets. We find a larger positive effect on performance in the imbalanced classification tasks. We show that, with a suitable hyper-parameter choice of the BROOD sampler, the BROOD-enhanced XGBoost model outperforms the regular XGBoost model on the DCG on the severely imbalanced data sets.

We discuss the similarities and differences with existing oversampling techniques. Although the purpose of BROOD sampling is different compared to existing minority oversampling techniques, we compare the performance of models that exploit BROOD samples sampled from the minority instances with those that exploit SMOTE, ADASYN and ROSE samples. We find that XGBoost models exploiting BROOD samples ~~are generally able to perform as well as or outperform~~ are at least able to attain a similar performance as these oversampling methods. Further, we discover that one can further enhance the performance of XGBoost models by exploiting the combination of artificial BROOD and ROSE samples ~~results in superior performances~~ on severely imbalanced data sets. With a suitable hyper-parameter choice of the ROSE and BROOD sampler, we find that the XGBoost model exploiting both ROSE and BROOD samples outperforms the regular XGoost model on the DCG in severely imbalanced classification tasks.

The current implementation of the BROOD sampler is able to handle multiple classes. Hence, for further research, we aim to investigate the use of unlabelled samples for multi-class classification tasks. Further, we aim to develop a suitable BROOD sampler that can handle categorical features without encoding and to apply our methodology in a cost-sensitive setting.

7. CRediT Authorship Contribution Statement

Van der Schraelen Lennert: Conceptualization, Methodology, Software, Validation, Formal analysis, Writing – original draft. **Stouthuysen Kristof**: Conceptualization, Writing – review & editing, Supervision. **Vanden Broucke Seppe**: Conceptualization, Writing – review & editing. **Verdonck Tim**: Conceptualization, Writing – review & editing, Supervision.

8. Declaration of Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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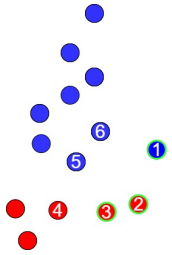
10. Appendix

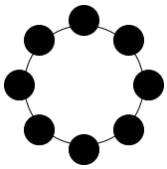
10.1. The BROOD Sampler

10.1.1. Visualization of the BROOD Sampler's steps

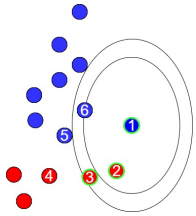
Figure 8 visualizes the different steps of the BROOD sampler on an artificial data set. In this example, $n_{\text{dir\_max}}$ is equal to 8, and we will sample from the data points 1, 2, and 3.



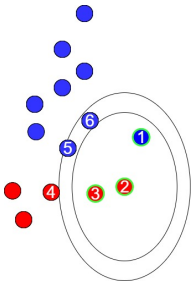
Step 1: Determine the data points from which we will sample. These data points have a green border in the plot.



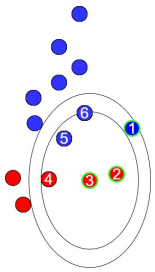
Step 2: We employ Mitchell's Best-Candidate algorithm to ensure that the sampled points are approximately uniformly distributed on the surface.



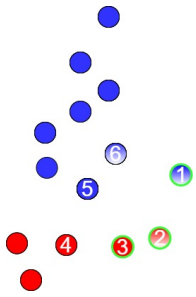
Step 3: We determine the neighborhoods of data point 1. The distance to point $(2, 6)$ is smaller than $2 \cdot \text{dist}_{\text{id\_ood}}$. The distance to the data point 3 is smaller than $2 \cdot \text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$.



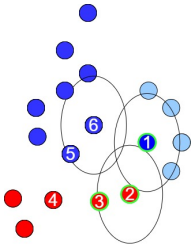
Step 3: We determine the neighborhoods of data point 2. The distance to the data points $(1, 3)$ is less than $2 \cdot \text{dist}_{\text{id\_ood}}$. The distance to points $(5, 6)$ is less than $2 \cdot \text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$.



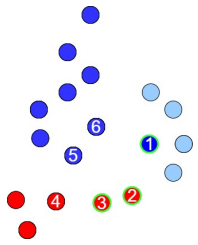
Step 3: We determine the neighborhoods of data point 3. The distance to the data points $(2, 4, 5, 6)$ is less than $2 \cdot \text{dist}_{\text{id\_ood}}$. The distance to point 1 is less than $2 \cdot \text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$.



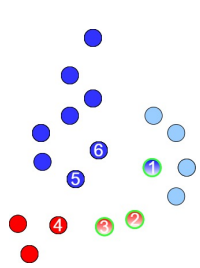
Step 4: We found that the data points $(2, 6)$ have a distance less than $2 \cdot \text{dist}_{\text{id\_ood}}$ from data point 1. We extract their data attributes.



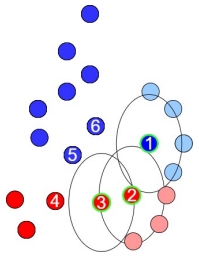
Step 5: We create artificial data points by sampling from data point 1. We keep the artificial data point if the distance from the data points $(2, 6)$ to the artificial data point is greater than $\text{dist}_{\text{id\_ood}}$.



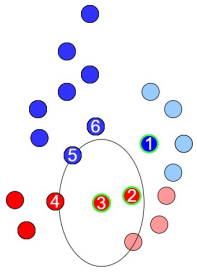
Step 6: We did not find any data points for this step.



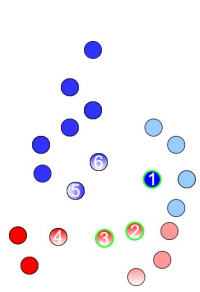
Step 4: We found that the data points $(1, 3)$ have a distance less than $2 \cdot \text{dist}_{\text{id\_ood}}$ from data point 2. We found that data point 3 has distance less than $2 \cdot \text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$, and we will sample from this data point in the future. We extract their data attributes.



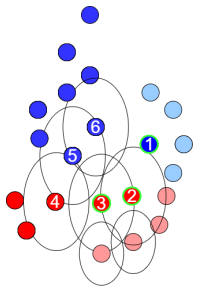
Step 5: We create artificial data points by sampling from data point 2. We keep the artificial data point if the distance from the data points $(1, 3)$ to the artificial data point is greater than $\text{dist}_{\text{id\_ood}}$.



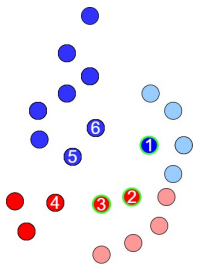
Step 6: The distance from data point 2 to data point 3 (same class, and we will sample from it in the future) is less than $2 \cdot \text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$. The distance from data point 3 to one artificial data point is less than $\text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$.



Step 4: We found that the data points $(2, 4, 5, 6)$ have a distance less than $2 \cdot \text{dist}_{\text{id\_ood}}$ from data point 3. Further, we found that the distance to one OOD sample is less than $\text{dist}_{\text{id\_ood}} + \text{dist}_{\text{ood}}$. We extract their data attributes.



Step 5: We create artificial data points by sampling from data point 3. We keep the artificial data point if the distance from the data points $(2, 4, 5, 6)$ to the artificial data point is greater than $\text{dist}_{\text{id\_ood}}$ and if the distance from the concerned artificial data point sampled from point 2 is less than dist_{ood}.



Step 6: We did not find any data points for this step.

Figure 8: Visualisation of the BROOD sampler's steps. Toy example created by the author that visualizes the working of the BROOD sampler.

10.1.2. Modifications

One can find the Python code of the BROOD sampler on Github[5]. We wrote a modification of the BROOD sampler that checks the class distribution of the ID data points with Mahalanobis smaller than one from the ID point from which we sample. In this case, we compare the local class distribution and the global class prior. The OOD samples receive the label for which the quotient between the local class distribution and the global class prior is the greatest.

Next, in the case that $\hat{\boldsymbol{h}}$ is class or instance dependent, the Euclidean distance between the OOD samples that are sampled from different points can differ. Hence, we propose a method that ensures that the Euclidean distance between the OOD samples remains the same. Focusing on BROOD(KNN), the sur-

[5] https://github.com/CFLDT/Regularization-Oversampling-for-Classification-Tasks-To-Exploit-What-You-Do-Not-Know

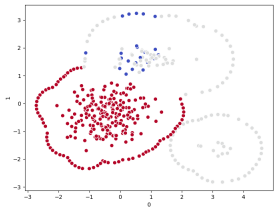
face area S_d^r of a d-dimensional hyper-sphere with radius r is given by [57]

$$S_d^r = \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1}. \tag{16}$$

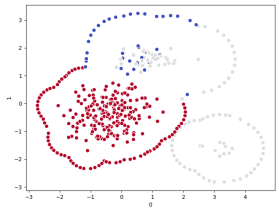
Denote with $S_d^{r\_\max}$ the surface of the hypersphere on which we sample directions from the instance with the highest d_{j_k}. We ensure that the number of directions that are created from an instance i equals

$$\frac{S_d^{r\_i}}{S_d^{\max\_r}} n_{\text{dir\_max}}. \tag{17}$$

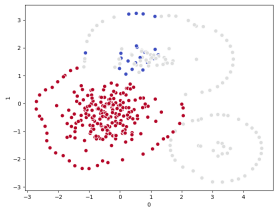
In figure 9, one finds a visualisation of the two modifications. One finds the BROOD(KNN) sampler on the top left. In this case, the artificially generated samples have the same label as the instance from which they are sampled. The local counterpart considers the labels of data points in the neighborhood of the data point from which they are sampled. The bottom pictures visualize the case where we use the BROOD(KNN) sampler with more equal distances between OOD samples.



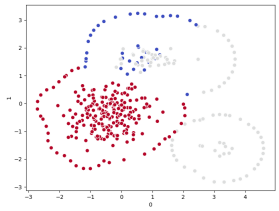
Visual of the standard BROOD(KNN) sampler.



Visual of local BROOD(KNN) sampler.



Visual of the standard BROOD(KNN) sampler with more equal distance between OOD samples.



Visual of local BROOD(KNN) sampler with more equal distance between OOD samples.

Figure 9: Visual comparison of the BROOD sampler's modifications. Comparison of the BROOD sampler's modifications in a multi-class setting on a toy data set.

10.2. General Overview of the Pipeline

As explained in the paper, we use random stratified sampling to obtain an initial train set consisting of 75% of all instances and a test set consisting of 25% of all instances. Furthermore, we split the initial train set (in a stratified way) into the final train set (50% of all instances) and a validation set (25% of all instances). We train the model on the final train set, use the validation set to optimize the models' hyper-parameters, and assess performance on the test set. We execute this procedure four times in a row for every data set, each time with a completely different test set. One can find a visual representation of the procedure in figure 10.

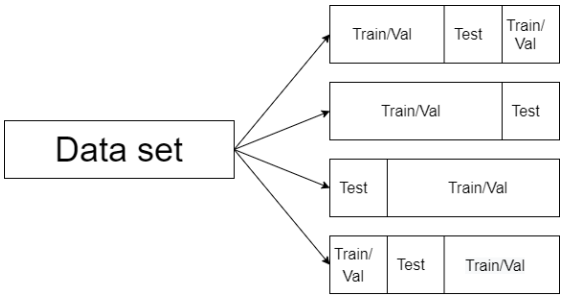


Figure 10: Visual representation of our cross-validation structure. We create four folds, each time with a completely different test set.

We apply a clever pipeline structure to ensure that the machine learning models can extract a maximal amount of information from the provided data sets. First, we create an additional dummy column for every numerical feature. If the numerical feature contains NaN values, the dummy column equals true on these positions. Further, in the numerical column, the NaN values are imputed by the median of the corresponding column. We treat the NaN values in categorical columns as an additional class.

Next, we use Weight Of Evidence (WOE) encoding to quantify the predictive power of each attribute [45]). The WOE value for attribute a in column c is given by

$$\text{WOE}_a^c = \log\left(\frac{((\text{ratio non-event in } a) + 0.5)/(\text{ratio non-event in } c)}{((\text{ratio event in } a) + 0.5)/(\text{ratio event in } c)}\right) \tag{18}$$

where we add 0.5 to handle missing events. The information value (IV) for column c is given by

$$\text{IV}^c = \sum_a \Big(\frac{((\text{ratio non-event in } a) + 0.5)}{(\text{ratio non-event in } c)} - \frac{((\text{ratio event in } a) + 0.5)}{(\text{ratio event in } c)}\Big)\text{WOE}_a^c. \tag{19}$$

From [45], if an attribute has IV value lower than 0.10, it is considered weak. To calculate the IV value for numerical features, we bin the numerical feature into 20 bins that contain approximately the same number of instances. We only keep informative features by deleting features with an IV value lower than 0.10. Further, if the number of features is greater than 30, we only keep the 30 most informative features with the highest IV value. In future steps, we use the WOE encoded values for categorical columns. Of course, as encodings require label information, these encodings are fitted on the train set. Unseen categorical attributes in the test or validation set have a WOE value of 0.

Subsequently, we standardize all features of the train set, and we apply the same scaler on the validation and test set. We

apply the BROOD sampler, with pre-determined parameters, to the train set.

Finally, we iterate over every possible combination of hyper-parameters for logistic regression and XGBoost models with and without artificially generated OOD samples. We test the performance of a model with a specific combination of hyper-parameters on the validation set. For instance, one can compare the ROC-AUC for every combination of hyper-parameters. We use the best model to predict the test set's instances and calculate the corresponding performance measures.

10.3. Overview of and Results on the Benchmark Data Sets

We use a validation set to pick an optimal combination of the set of hyper-parameters. The set of hyper-parameters can be found in table 5. One can find the performance metrics of our models in table 6. These values were used to create figure 4.

10.4. Overview of and Results on the Severely Imbalanced Data Sets

We use a validation set to pick an optimal combination of the set of hyper-parameters. The set of hyper-parameters can be found in table 7. One can find the performance metrics of our models on the severely imbalanced data sets in table 10. These values were used to create figures 5 and 6.

Method	Logit	XGBoost	XGBoost_BROOD
β_t	/	/	[1]
c_{ood_1}	/	/	[0, 0.50, 1, 2, 10]
c_{ood_0}	/	/	[0, 0.50, 1]
L2-Regularisation	[0, 0.10, 1, 10]	[0, 10, 100]	[0, 10, 100]
Max Tree Depth	/	[5, 10]	[5, 10]
# Estimators	/	[50, 200]	[50, 200]
Subsample	/	[0.25, 0.50, 0.75]	[0.25, 0.50, 0.75]
Learning Rate	[0.10]	[0.10]	[0.10]

Table 5: List of hyper-parameters for the benchmark data sets. We iterate over these list during cross-validation to find the optimal combination.

Method	Logit	XGBoost	XGB_BR(ALL_ROT)	XGB_BR(ALL_KNN)
UCI Ecoli	0.932	0.953	**0.967**	0.959
UCI Mammographic Masses	**0.870**	0.865	0.854	0.857
UCI Sonar	0.776	0.864	**0.912**	0.878
UCI Ionosphere	0.899	0.969	0.976	**0.984**
UCI Breast Cancer Wisconsin	**0.993**	0.991	0.993	0.987
UCI Heart	0.893	0.881	0.886	**0.895**
UCI Indian Liver Patient	0.749	0.731	**0.753**	0.746
UCI Liver Disorders	**0.673**	0.593	0.644	0.627
UCI Breast Cancer	**0.692**	0.653	0.655	0.684
UCI Vehicle	0.988	**0.995**	0.985	0.992
UCI Contraceptive method	0.732	**0.740**	0.737	0.739
UCI German Credit Card	0.778	**0.785**	0.779	0.765
UCI Credit Approval	0.928	0.937	0.935	**0.938**
UCI Bank Marketing	0.934	0.938	0.938	**0.940**
UCI Madelon	0.629	**0.857**	0.835	0.850

ROC-AUC of the benchmark data sets.

Method	Logit	XGBoost	XGB_BR(ALL_ROT)	XGB_BR(ALL_KNN)
UCI Ecoli	0.798	0.851	**0.863**	0.852
UCI Mammographic Masses	**0.831**	0.810	0.807	0.808
UCI Sonar	0.772	0.868	**0.920**	0.885
UCI Ionosphere	0.890	0.961	0.970	**0.976**
UCI Breast Cancer Wisconsin	0.991	0.989	**0.991**	0.987
UCI Heart	0.885	0.875	0.878	**0.888**
UCI Indian Liver Patient	0.495	0.483	0.521	**0.526**
UCI Liver Disorders	**0.505**	0.443	0.473	0.492
UCI Breast Cancer	0.489	0.443	0.451	**0.491**
UCI Vehicle	0.961	**0.984**	0.971	0.974
UCI Contraceptive method	0.434	0.467	0.469	**0.476**
UCI German Credit Card	0.585	0.591	**0.607**	0.596
UCI Credit Approval	0.914	0.921	0.916	**0.924**
UCI Bank Marketing	0.609	0.638	0.635	**0.647**
UCI Madelon	0.579	**0.849**	0.825	0.848

AP of the benchmark data sets.

Method	Logit	XGBoost	XGB_BR(MIN_ROT)	XGB_BR(MIN_KNN)
UCI Ecoli	4.087	4.408	**4.529**	4.504
UCI Mammographic Masses	**18.248**	18.239	18.070	18.041
UCI Sonar	6.496	7.228	**7.607**	7.429
UCI Ionosphere	8.067	8.787	8.794	**8.896**
UCI Breast Cancer Wisconsin	12.939	12.894	12.983	**13.025**
UCI Heart	7.746	7.489	**7.792**	7.761
UCI Indian Liver Patient	5.299	5.458	6.062	**6.133**
UCI Liver Disorders	**4.487**	3.823	4.046	4.336
UCI Breast Cancer	3.511	3.137	3.218	**3.566**
UCI Vehicle	12.075	**12.256**	12.237	12.060
UCI Contraceptive method	8.637	**9.379**	9.283	9.246
UCI German Credit Card	10.353	10.552	10.422	**10.565**
UCI Credit Approval	15.231	**15.398**	15.277	15.314
UCI Bank Marketing	14.209	14.674	14.866	**14.873**
UCI Madelon	29.449	**40.607**	40.011	40.394

DCG of the benchmark data sets.

Table 6: Performance metrics of the machine learning models on the benchmark data sets. We use BROOD(ALL_ROT) ($n_{\text{dir\_max}}$ = 30, $n_{\text{dir\_samp}}$ = 90, $\text{dist}_{\text{id\_ood}}$ = 4) and BROOD(ALL_KNN) ($n_{\text{dir\_max}}$ = 30, $n_{\text{dir\_samp}}$ = 90, $\text{dist}_{\text{id\_ood}}$ = 1.5) to generate BROOD samples. The best-performing model is in bold. The best-performing model is in bold. We abbreviate 'XGBoost' as ' XGB' and 'BROOD' as 'BR'.

Method	Logit	XGBoost	XGBoost_BROOD
β_t	/	/	[1]
c_{ood_1}	/	/	[0, 1, 2, 5, 10, 100, 1,000]
c_{ood_0}	/	/	/
L2-Regularisation	[0, 0.10, 1, 10]	[0, 10, 100]	[0, 10, 100]
Max Tree Depth	/	[5, 10]	[5, 10]
# Estimators	/	[50, 200]	[50, 200]
Subsample	/	[0.25, 0.50, 0.75]	[0.25, 0.50, 0.75]
Learning Rate	[0.10]	[0.10]	[0.10]

Table 7: List of hyper-parameters for the severely imbalanced data sets. We iterate over these list during cross-validation to find the optimal combination.

Method	Logit	XGBoost	XGBoost_SMOTE	XGBoost_ADASYN	XGBoost_ROSE
ESA Polish Bankruptcy	0.852	0.892	0.906	0.902	0.900
Financial Distress	0.913	0.912	0.922	0.920	0.911
UCI German Credit Card IMB	0.774	**0.805**	0.773	0.763	0.783
UCI Credit Approval IMB	0.908	0.930	0.915	0.941	0.936
UCI Bank Marketing IMB	0.897	0.917	0.925	**0.926**	0.910
IBM Telco Customer Churn	0.817	0.591	0.629	0.638	0.642
ETL Credit Card Approval	0.618	0.597	0.592	0.586	0.635
VUB Credit Scoring	0.775	**0.784**	0.753	0.759	0.763
KDD Cup 1998	0.528	0.517	0.526	0.532	0.519
(Priv.) Car Insurance Fraud	0.677	0.708	0.707	0.717	0.718
(Priv.) APATA Credit Card Fraud	0.810	0.500	0.500	0.500	0.500
JAR Financial Statement Fraud	0.708	0.728	0.718	0.716	0.714
IEEE-CIS Cus. Trans. Fraud	0.768	0.828	0.770	0.753	0.783
Synt. Mobile Trans. Fraud	0.948	0.993	0.990	0.984	0.993
Synthetic Credit Card Fraud	0.980	0.981	0.981	**0.987**	0.983

Method	XGB_BR(MIN_ROT)	XGB_BR(MIN_KNN)	XGB_ROSE_BR(MIN_ROT)	XGB_ROSE_BR(MIN_KNN)
ESA Polish Bankruptcy	0.895	**0.908**	0.891	0.897
Financial Distress	0.915	0.915	0.921	**0.931**
UCI German Credit Card IMB	0.766	0.764	0.734	0.782
UCI Credit Approval IMB	0.928	**0.947**	0.929	0.945
UCI Bank Marketing IMB	0.912	0.923	0.911	0.918
IBM Telco Customer Churn	**0.820**	0.820	0.814	0.819
ETL Credit Card Approval	0.599	0.581	0.589	**0.629**
VUB Credit Scoring	0.777	0.776	0.773	0.771
KDD Cup 1998	0.536	0.527	0.533	**0.541**
(Priv.) Car Insurance Fraud	0.699	0.690	**0.761**	0.751
(Priv.) APATA Credit Card Fr.	**0.853**	0.708	0.655	0.808
JAR Financial Statement Fr.	0.719	0.730	0.729	**0.737**
IEEE-CIS Cus. Trans. Fraud	0.825	**0.839**	0.778	0.769
Synth. Mobile Trans. Fr.	**0.992**	0.989	0.989	0.991
Synthetic Credit Card Fraud	0.983	0.985	0.982	0.985

ROC-AUC of the severely imbalanced data sets

Method	Logit	XGBoost	XGBoost_SMOTE	XGBoost_ADASYN	XGBoost_ROSE
ESA Polish Bankruptcy	0.476	0.630	0.632	0.619	0.618
Financial Distress	0.313	**0.400**	0.384	0.366	0.389
UCI German Credit Card IMB	0.271	0.299	0.286	0.282	**0.321**
UCI Credit Approval IMB	0.561	0.571	0.576	**0.629**	0.616
UCI Bank Marketing IMB	0.239	**0.294**	0.278	0.268	0.292
IBM Telco Customer Churn	0.226	0.110	0.126	0.137	0.132
ETL Credit Card Approval	0.053	0.041	0.022	0.030	0.052
VUB Credit Scoring	0.129	0.127	0.121	0.128	0.125
KDD Cup 1998	0.059	0.058	0.058	**0.061**	0.055
(Priv.) Car Insurance Fraud	0.068	0.064	0.069	0.075	0.073
(Priv.) APATA Credit Card Fraud	0.052	0.008	0.008	0.008	0.008
JAR Financial Statement Fraud	0.072	0.084	0.079	0.073	0.071
IEEE-CIS Cus. Trans. Fraud	0.289	0.322	0.237	0.245	0.310
Synt. Mobile Trans. Fraud	0.678	0.880	0.856	0.881	0.898
Synthetic Credit Card Fraud	0.797	0.839	0.845	0.853	0.866

Method	XGB_BR(MIN_ROT)	XGB_BR(MIN_KNN)	XGB_ROSE_BR(MIN_ROT)	XGB_ROSE_BR(MIN_KNN)
ESA Polish Bankruptcy	0.623	**0.648**	0.622	0.629
Financial Distress	0.392	0.383	0.400	0.388
UCI German Credit Card IMB	0.275	0.282	0.272	0.273
UCI Credit Approval IMB	0.608	0.609	0.559	0.613
UCI Bank Marketing IMB	0.211	0.265	0.248	0.275
IBM Telco Customer Churn	0.232	**0.233**	0.228	0.228
ETL Credit Card Approval	0.051	0.037	0.050	**0.078**
VUB Credit Scoring	0.124	0.126	0.123	**0.131**
KDD Cup 1998	0.058	0.057	0.058	0.060
(Priv.) Car Insurance Fraud	0.087	0.074	**0.111**	0.086
(Priv.) APATA Credit Card Fr.	**0.256**	0.178	0.147	0.171
JAR Financial Statement Fr.	0.084	0.083	0.095	**0.096**
IEEE-CIS Cus. Trans. Fraud	0.325	**0.343**	0.297	0.298
Synth. Mobile Trans. Fr.	0.878	0.890	0.907	**0.910**
Synthetic Credit Card Fraud	**0.884**	0.875	0.880	0.869

AP of the severely imbalanced data sets

Method	Logit	XGBoost	XGBoost_SMOTE	XGBoost_ADASYN	XGBoost_ROSE
ESA Polish Bankruptcy	9.312	10.788	10.803	10.795	10.796
Financial Distress	3.363	4.480	4.497	4.174	4.404
UCI German Credit Card IMB	1.679	2.028	2.049	1.779	**2.104**
UCI Credit Approval IMB	2.097	1.966	2.128	2.126	**2.232**
UCI Bank Marketing IMB	2.039	2.605	2.486	2.486	**2.779**
IBM Telco Customer Churn	5.293	4.005	4.035	4.589	3.654
ETL Credit Card Approval	0.408	0.520	0.322	0.398	0.733
VUB Credit Scoring	5.431	4.992	5.140	5.228	5.435
KDD Cup 1998	2.104	1.984	2.003	**2.221**	1.705
(Priv.) Car Insurance Fraud	2.541	2.288	2.400	2.885	2.527
(Priv.) APATA Credit Card Fraud	0.000	0.000	0.000	0.000	0.000
JAR Financial Statement Fraud	2.023	2.703	2.384	2.210	2.329
IEEE-CIS Cus. Trans. Fraud	8.463	9.191	7.698	7.939	8.889
Synth. Mobile Trans. Fraud	5.282	6.519	6.610	6.693	6.720
Synthetic Credit Card Fraud	7.600	7.628	7.644	7.803	7.964

Method	XGB_BR(MIN_ROT)	XGB_BR(MIN_KNN)	XGB_ROSE_BR(MIN_ROT)	XGB_ROSE_BR(MIN_KNN)
ESA Polish Bankruptcy	10.851	10.936	10.846	**10.989**
Financial Distress	4.562	4.464	**4.696**	4.255
UCI German Credit Card IMB	1.774	1.707	1.906	1.830
UCI Credit Approval IMB	2.151	2.072	2.049	2.072
UCI Bank Marketing IMB	1.902	2.241	2.321	2.592
IBM Telco Customer Churn	5.344	5.359	**5.674**	5.662
ETL Credit Card Approval	0.590	0.465	0.677	**0.955**
VUB Credit Scoring	5.050	5.116	5.109	**5.771**
KDD Cup 1998	1.949	1.698	2.218	1.967
(Priv.) Car Insurance Fraud	3.217	2.764	**4.002**	2.911
(Priv.) APATA Credit Card Fr.	**2.086**	1.572	1.562	1.580
JAR Financial Statement Fr.	3.073	2.842	**3.258**	3.130
IEEE-CIS Cus. Trans. Fraud	9.290	**9.560**	8.888	8.971
Synth. Mobile Trans. Fr.	6.720	6.705	6.670	**6.794**
Synthetic Credit Card Fraud	8.104	8.034	**8.155**	8.019

DCG of the severely imbalanced data sets

Table 10: Performance metrics of the machine learning models on the severely imbalanced data sets We use BROOD(MIN_ROT) ($n_{\text{dir\_max}}$ = 30, $n_{\text{dir\_samp}}$ = 90, $\text{dist}_{\text{id\_ood}}$ = 4) and BROOD(MIN_KNN) ($n_{\text{dir\_max}}$ = 30, $n_{\text{dir\_samp}}$ = 90, $\text{dist}_{\text{id\_ood}}$ = 1.5) to generate BROOD samples. We use the imbalance ratio that on average performs best on all data sets. The stand alone SMOTE, ADASYN, and ROSE samplers aim to achieve an imbalance ratio of 0.20. The ROSE sampler along with the BROOD sampler aim to achieve an imbalance ratio of 0.10. The best-performing model is in bold. We abbreviate 'XGBoost' as ' XGB' and 'BROOD' as 'BR'.