

# Datamap-Driven Tabular Coreset Selection for Classifier Training

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## ABSTRACT

In the era of data-driven decision-making, efficient machine learning model training is crucial. We present a novel algorithm for constructing *tabular data* coresets using datamaps created for Gradient Boosting Decision Trees models. The resulting coresets, computed within minutes, consistently outperform other baselines and match or exceed the performance of models trained on the entire dataset. Additionally, a training enhancement method leveraging datamap insights during the inference phase improves performance with mathematical guarantees, given a defined property holds. An explainability layer and tools for coreset size optimization further enhance the efficiency of training tabular machine learning models.

## 1 INTRODUCTION

In data science, successful model training is essential for decision-making and predictive analytics. This involves handling extensive training data and carefully selecting appropriate machine learning (ML) models while optimizing their configurations. However, finding the most suitable model and optimal configuration can be time-consuming due to numerous training iterations. To tackle this issue, various algorithms have been introduced to generate a condensed subset of data, referred to as a *coreset*. Initially developed for clustering tabular data [22], and found extensive applications in recent computer vision tasks (e.g., [32]). However, the application of coresets in the context of tabular data remains relatively limited, and mainly focused on coresets that are tailored to classical ML algorithms [26, 31, 38, 42]. Although these works provide guarantees for their usage within the designated classic models, they have limited coverage for the advanced models commonly used in tabular data domain, such as XGBoost [14] or TabNet [9].

**Goal.** Focusing on classification models, our goal is to create a tabular coreset that achieves high performance on advanced ML models, and could take as an input any type of tabular data (numeric, categorical, etc.). As opposed to some of the previous work, the selected coreset is of a size that the user has provided, and the coreset remains relevant after the addition of new features, which happen frequently during the feature engineering process.

**Intuition Behind Our Solution.** Our solution draws inspiration from decision trees based ML classification algorithms, where the leaves serve as sets that, once the tree is constructed, contain all the examples the model was trained on. During inference, these leaves or the union of leaves (in case of multiple trees) determine the classification of unseen examples, assigning the same label to all examples within one leaf. Our algorithm capitalizes on the observation that leaves containing many examples, all belonging to the same label, can be viewed as forming equivalence classes. As a result, the algorithms can effectively classify similar instances without the need to train on all these examples. Leveraging this insight, we can select a coreset comprising only a small subset of these examples

while excluding the others. However, identifying these *easy to learn* and *hard to learn* regions is non-trivial due to potential variations in splits by different decision trees and the impact of different sampling strategies, leading to diverse leaf nodes and varying results.

**Proposed Solution.** Our approach addresses the concern by introducing an algorithm for creating a tabular datamap, originally designed for the textual domain [37]. The datamap identifies regions in the data that are easy or hard to learn during model training. We then develop an algorithm that utilizes the datamap to select a coreset, encompassing hard-to-learn regions and small representatives of easy-to-learn ones. To the best of our knowledge, this is the first application of datamaps for this purpose. This innovative strategy results in a coreset that competes in terms of performance with even complex models trained on the entire dataset. Our efficient implementation, CoreTab, constructs coresets within minutes even for sizable datasets, outperforms competitors in speed and achieves better quality results, up to a 30% increase in some cases compared to the best performing baseline. Additionally, we offer an explainability layer to help users understand the inclusion or condensation of specific data sections in the coreset.

**Example 1.1.** Consider our approach applied to the *BankLoan* dataset. Here, the goal is to train an ML model for classifying loan approval (*True*) or rejection (*False*) based on various attributes. Imagine a decision tree leaf containing 10% of the data, where all examples share the label *False*. Examining the decision tree path leading to this leaf reveals conditions  $bank\_credit \leq 200$  and  $Bankruptcies \geq 1$ , defining a specific region within the dataset. This region is homogeneous, making predictions easy due to a consistent label. Sampling a small subset from this *easy-to-learn* region is likely highly representative. Conversely, challenging regions for the model require more data. Thus, we create a datamap partitioning the data space into regions of varying complexity based on label homogeneity and the model’s ease or difficulty in making predictions within each region.

**Training Enhancement.** Leveraging the valuable insights encoded within the generated datamap, we introduce an innovative approach to enhance the ML model training process. Our aim is to streamline this intricate and resource-intensive process, particularly beneficial when repeated model training is necessary ([23]). We propose a method that significantly improves the performance of models trained on the coreset, often matching or surpassing the performance of models trained on the entire dataset. Moreover, this method provides insights into the trade-offs in results, supported by mathematical guarantees (Section 5), contingent upon a defined property of the data and model. These benefits extend to hyperparameter tuning and cross-validation, both requiring numerous training iterations ([45]). To achieve this, we leverage the datamap, a byproduct of the CoreTab algorithm, during the inference phase of a model trained on the coreset. As the datamap algorithm exclusively uses the training set, we achieve a performance boost without data leakage concerns.

Our system also includes an investigation tool for users to explore coreset size and accuracy trade-offs, facilitating the selection of the most appropriate coreset size based on desired quality preservation.

*Contributions.* This work presents several contributions:

- (1) Introduction of an *advanced algorithm tailored for creating a tabular datamap*, a crucial element in our coreset generation process, specifically designed for Gradient Boosting Decision Trees (GBDT) models.
- (2) Proposal of a *novel algorithm and problem formulation for creating coresets using a datamap* for tabular data, addressing the challenge of efficient coreset creation. This includes an explainability layer to understand patterns within the coreset compared to the full dataset.
- (3) Unique approach for *training enhancement* by leveraging the datamap during the inference phase of a model trained over the coreset, supported by theoretical guarantees for model performance. It also includes an explainability layer for optimal coreset size determination.
- (4) Provision of *comprehensive experimental results* demonstrating the high performance of CoreTab across various models and datasets, along with thorough comparisons with various baseline methods for tabular coreset selection. Additionally, showcasing the benefits of our approach for training enhancement, revealing significantly reduced training times and high model performance.

## 2 RELATED WORK

Our work relates to two research areas: (1) data sampling and summarization, and (2) coreset and instance selection techniques. In this section, we highlight distinctions from existing methods and present comparison results in Section 6.

*Row Sampling and Data Summarization.* Row sampling is widely used in various domains, such as Approximate Query Processing (AQP) for expediting query results [7, 10] and data visualization for reducing data points [34]. Greedy algorithms are applied for query result diversification [30, 41]. In contrast, our ML model optimization focuses on selecting rows based on labels and their relevance. In AutoML, [28] uses genetic algorithms for a compact and representative data subset, emphasizing general data characteristics. Unlike our label-centric approach, it aims for versatility. In Data Summarization, techniques like dimensionality reduction [19] or data sketches for online streams [16] produce compressed versions. While useful for AQP and feature engineering [19], they are unsuitable for ML model training, where access to actual data is crucial.

*Fundamentals of Coresets and Instance Selection.* Initially called Instance Selection ([29]), these techniques involve selecting, generating, and transforming instances to enhance data mining algorithms. Coresets, also known as representative subsets or summarization methods, efficiently approximate complex datasets while retaining crucial structural insights. Works like [22] for clustering tabular data and [20] for statistical mixture models introduced coresets to reduce data size. Notably, these works primarily focus on unsupervised settings, preserving data characteristics without labels.

*Recent Coresets Work.* The CRAIG method [32], a foundational technique for selecting supervised ML model coresets that closely approximate the full gradient, was initially introduced for computer vision applications. Subsequent works have built on this foundation, also focusing primarily on computer vision [11, 33, 35, 39]. While these methods are not directly applicable to tabular data, we adapted the current state-of-the-art coreset selection method for computer vision [44] and compared our algorithm to it in Section 6.

Recent works for tabular data have focused on coreset selection for clustering tasks ([12, 15, 25, 40]). These clustering-centric approaches may not capture patterns necessary for classification tasks. Additionally, methods for tabular classification coresets ([26, 31, 38]), primarily tailored to basic ML algorithms, were comprehensively evaluated in our research, highlighting the superior efficacy of our coreset generation approach (Section 6).

While prior work has developed coresets for relational databases ([13, 42]), primarily relying on gradient change principles, our research emphasizes creating subsets guided by datamaps from Gradient Boosting Decision Tree (GBDT) models. Datamap-informed coresets show high versatility and applicability across complex ML models (Section 6), making our approach suitable for a wide range of tabular data scenarios. We excluded the comparison to [42] because, as the authors noted, it represents an approximation of the CRAIG algorithm designed for multiple tables. Even when applied to a single table, this algorithm remains an approximation. The authors contend that for single table scenarios, the exact CRAIG algorithm would provide superior performance.

## 3 PRELIMINARY

In this section, we establish the groundwork for our upcoming algorithm, both for tabular coresets and tabular datamaps, and discuss essential components of Gradient Boosting Decision Tree (GBDT) algorithms, pivotal to creating datamaps.

*Problem Formulation.* In line with standard ML conventions, we consider a dataset  $D$  with  $[R_1, \dots, R_N]$  rows and  $[C_1, \dots, C_M]$  columns drawn from distribution  $\mathcal{D}$ . A coreset is a subset of rows of  $D$ , projected over all columns ([22]).

*Definition 3.1 (Tabular Coreset).* For a dataset  $D$  with row-indices  $R$  and column indices  $C$ , a tabular coreset of size  $n \times m$  is denoted as  $d$  and is defined as  $D[r, C]$  for any  $r \in [R]^n$ . Here,  $[R]^n$  represents the set of all  $n$ -subsets of  $R$ , i.e.,  $[R]^n = \{R' \mid (R' \subseteq R) \wedge (|R'| = n)\}$ .

We focus on binary classification ML models with  $P$  and  $N$  as the positive and negative classes, respectively. In a typical scenario, a data scientist trains an ML model  $M$  using configuration  $conf$  to predict labels of the dataset  $D$ , defined in the training as column  $y$ . We denote this model as  $M(D, y, conf)$ . Let  $Rec(M(D, y, conf))$  and  $Prec(M(D, y, conf))$  represent the recall and precision of the trained model, with  $Acc(M(D, y, conf))$  being the classification metric to optimize (e.g., recall, precision, F1-score). Next, we introduce two methods for optimizing coreset creation.

*Definition 3.2 (Coreset Creation Optimizations).* The coreset creation could be optimized based on the following:

- **[Opt\_per] Optimization based on models performance:** Given  $\Delta_{Recall}$ ,  $\Delta_{Precision}$ , a thresholds for performance guarantees, derive the minimal size  $n$  and a coreset  $d$  of size  $n$ , s.t.  $n \ll N$ , s.t.

$$\forall M: \text{Rec}(M(d, y, \text{conf})) - \Delta_{\text{Recall}} \geq \text{Rec}(M(D, y, \text{conf}))$$

$$\text{Prec}(M(d, y, \text{conf})) - \Delta_{\text{Precision}} \geq \text{Prec}(M(D, y, \text{conf}))$$

- **[Opt\_size] Optimization based on coreset size:** Given  $n$ , the coreset's  $d$  size, find the coreset  $d^* \in [R]^n$  s.t.  $\text{Acc}(M(d^*, y, \text{conf})) \geq \text{Acc}(M(d, y, \text{conf})), \forall d \in [R]^n$ .

*Goal.* The objective of our algorithm, *CoreTab*, is to choose a tabular coreset that minimizes training computation times for a given ML model, without compromising the original performance or even improving it. The algorithm optimizes coreset creation according to both methods, accommodating user preferences.

*Tabular Datamaps.* The Datamap concept, initially introduced in Natural Language Processing (NLP) [37], provides a distinctive view of how ML models perceive and adapt to data during training. It maps and diagnose datasets as they evolve, offering insights into the impact of different data samples on the learning process. In NLP, it creates a map with regions, each representing a set of words and indicating the complexity of learning their representation by the model. Adapting the Datamap concept to tabular data necessitates a shift from neural network-centric gradient changes to delineating regions based on data characteristics (columns values). Unlike NLP models, tabular data includes labels for each row, crucial for model construction. The goal is to capture groups perceived as similar or equivalent by ML models, emphasizing features essential for accurate label-based segregation. Each row is assigned to a region based on similarity within crucial features. We denote the number of examples in a region as its *size*.

*Definition 3.3 (Group Homogeneity).* Given a threshold value  $\psi$ , denote  $g$  a group of tuples each labeled by either  $N$  or  $P$ . We define  $g_n$  and  $g_p$ , as the set of tuples with the label  $N$  and  $P$ , respectively. A group is considered homogeneous concerning the label column if either of the following conditions is met: The proportion of tuples with label  $N(P)$  in the group, denoted as  $\frac{|g_n|}{|g|}$  ( $\frac{|g_p|}{|g|}$ ), is greater than or equal to  $\psi$ .

In summary, the devised datamap divides the original dataset into smaller groups, each characterized by the resemblance of several attributes considered meaningful for distinguishing data points based on their labels. It is crucial to emphasize that not all regions have substantial sizes, and not all regions exhibit homogeneity according to predefined thresholds. Adapting the terminology from the original datamap to our case, we refer to regions as *easy to learn* if they are both homogeneous and large based on two thresholds (one for homogeneity and one for size). Conversely, non-homogeneous groups are labeled as *hard-to-learn* since the ML model struggles to segregate the data points within these regions into homogeneous groups. Lastly, there are other regions, specifically small homogeneous ones, designated as *ambiguous* to the model. This implies that the model succeeded in separating the data points into homogeneous regions within these areas, but the challenge was mitigated by their small size. The larger the groups, the more closely they align with the *easy-to-learn* regions. For brevity, the regions referred as *easy*, *hard*, *amb*. The subsequent section elucidates the primary reasons why these traits define the level of data complexity for the model, with further emphasis in Algorithm 1. Formally,

*Definition 3.4 (Tabular Datamap).* We define a Tabular Datamap  $dm$  with  $k$  non-overlapping regions as  $dm = f_1, \dots, f_k, [r_{i_1}, \dots, r_{i_j}] \in$

$f_i$ , where  $1 \leq j \leq N$ , and  $f_i \cap f_j = \emptyset$  for all  $i \neq j \in [1, k]$ . Each region  $f_i$  is characterized by a set of rules that define its boundaries. Each rule consists of an attribute (from the data space  $\mathcal{D}$ ) and a valid value range for that attribute. Formally,  $f_i = \{(c_{i_1}, \text{val}_{i_{j_1}}, \text{val}_{i_{j_2}}), \dots, (c_{i_j}, \text{val}_{i_{j_1}}, \text{val}_{i_{j_2}})\}$ . Each data entry  $r_p \in \mathcal{D}$  could be assigned to exactly one region based on the region's defined boundaries. This assignment occurs when the attribute values of the entry satisfy the rules of the regions. Formally,  $r_p \in f_j \rightarrow \text{val}_{j_{b_1}} \leq r_p[c_{j_b}] \leq \text{val}_{j_{b_2}}, \forall (c_{j_b}, \text{val}_{j_{b_1}}, \text{val}_{j_{b_2}}) \in f_j$ . The types of regions are defined using homogeneity (defined in Section 4), and the size of the region (denoted as  $|f_i|$ ):

$$\text{easy\_to\_learn} = \{f_i | (\text{homogenous}(f_i, \psi) = \text{True}) \& (|f_i| \geq \tau)\}$$

$$\text{hard\_to\_learn} = \{f_i | (\text{homogenous}(f_i, \psi) = \text{False})\}$$

$$\text{ambiguous\_to\_learn} = \{f_i | (\text{homogenous}(f_i, \psi) = \text{True}) \& (|f_i| \leq \tau)\}$$

*Gradient Boosting Decision Trees Utilization.* Next, we explain the use of *Gradient Boosting Decision Tree* (GBDT) principles to construct tabular datamaps and how they facilitate coreset selection (explained in Section 4). GBDT, a powerful ensemble learning technique introduced in [21], and is widely adopted in popular algorithms such as XGBoost [14]. GBDT iteratively creates a series of decision trees, forming additive regression models. The algorithm, in each iteration, fits a parameterized function (the base learner) to minimize "pseudo"-residuals, derived from a specific loss function. By aggregating predictions from these trees, it steadily improves predictive accuracy. The formal algorithm is omitted for brevity. To create datamaps with essential attributes (explained earlier), we use weak learners, specifically the trees generated during GBDT's initial phases. We intentionally limit the number of trees, encouraging the emergence of distinct groups characterized by properties relevant to at least one weak learners.

Our algorithm leverages the unique features of gradient boosting trees. These trees start with a shallow initial tree and use its predictions to guide the construction of subsequent trees by calculating error gradients. Each tree is divided into leaves, representing clusters of data with similar attributes, often related to label columns. Some clusters are completely homogeneous, meaning the model makes no errors on these samples, while others may have multiple labels, presenting challenges. In later trees, non-homogeneous clusters are refined, reducing error rates. Regions that remain non-homogeneous in later trees pose challenges to the algorithm's learning process and are included in the coreset.

## 4 CORESET AND DATAMAP ALGORITHMS

This section explores *CoreTab*, a system designed for constructing a coreset from the original data. Here, we focus on coreset creation based on user-defined size optimization (*opt\_size*), while the subsequent section discusses coreset creation based on performance optimization (*opt\_per*). We start by elucidating the algorithm (Algorithm 1) responsible for crafting a datamap, a pivotal element in the coreset selection process. Next, we delve into the algorithm (Algorithm 2) generating tabular coresets, leveraging the datamap as a foundational component, focusing on the *hard* regions.

### 4.1 Tabular Datamap Creation

We delve into the core stages of tabular datamap generation, fully detailed in Algorithm 1. This algorithm adopts an *Optimizing Based*

on *Labels* approach, giving priority to constructing the datamap primarily guided by data point labels. In practical scenarios, a weak learner, typically represented by a decision tree, may fail to accurately classify some data points, resulting in mixed-label leaves that eventually form the examined regions. To mitigate this, a threshold is set for the required homogeneity of a region concerning the label, as formally defined in Section 3.

*Initialization.* The algorithm’s inputs are the Dataset  $D$ , the number of trees for GBT algorithm, and the threshold for the size of the considered regions, named as groups. As explained in Section 6, we have carefully chosen the default values for those parameters, that work best on a wide variety of datasets and tasks. However, the user could change them according to his needs. Then, the GBDT algorithm is run for the given number of trees, and store the resulted trees in *trees* parameter. Another part of the initialization is creation of two sets of sets. The first, denoted as *datamap* is initialized as an empty set, and will eventually contain the datamap of the GBT algorithm. The second set of sets, denoted as *data\_groups*, contains initially a set of all the data points in the given dataset and will be used for storing the intermediate calculated groups to be added later to the datamap, upon reaching certain criterion.

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#### Algorithm 1 Creation of Datamap

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**Input:** Original Dataset  $D$ ,  $t_{num} = 30$ ,  $\tau = 5$   
**Output:** *datamap*

```

initialization: trees = GBT(data =  $D$ , #trees =  $t_{num}$ )
datamap = []
data_groups =  $[[r_1, \dots, r_N]]$ 
for every tree  $t \in [t_1, t_{t_{num}}]$  do
    leaves = leaves( $t$ )
    new_data_groups = []
    for every group in the data_groups do
        for every leaf in leaves do
            if  $leaf \cap group \neq \emptyset$  then
                add  $leaf \cap group$  to new_data_groups
            end if
        end for
    end for
    data_groups = new_data_groups
    for group  $\in$  data_groups do
        if  $(|group| \leq \tau) \vee (homogeneous(group) = True)$  then
            add group to datamap
            remove group from data_groups
        end if
    end for
end for
add data_groups to datamap
return datamap

```

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*Leveraging Gradient Boosting Decision Trees.* We iterate through each tree generated in the initial phase of the Gradient Boosting Decision Trees (GBDT) algorithm, and store its leaves in the *leaves* parameter. Additionally, we initialise an empty set *new\_data\_groups* for each tree that will hold the newly formed groups (as explained next). For each group within *data\_groups*, we check whether a

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#### Algorithm 2 CoreTab Algorithm - tabular coresets selection

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**Input:** Training Set  $S$ , coreset size  $n$ ,  $t_{num} = 30$ ,  $\tau = 5$ , *samp\_ratio*  
**Output:**  $d = [r_{i_1}, r_{i_2}, \dots, r_{i_n}]$  coreset of size  $n$

```

coreset = []
datamap = datamap_creation( $S$ ,  $t_{num}$ ,  $\tau$ )
for region  $\in$  datamap do
    if homogeneous(region) = False then
        coreset.append(region  $\cap S$ )
    end if
end for
if sizeoff(coreset)  $\geq n$  then return coreset
end if
easy_to_learn_candidates = []
for region  $\in$  datamap do
    if homogeneous(region) = True then
        easy_to_learn_candidates.append(region  $\cap S$ )
    end if
end for
for region  $\in$  sort_by_size_desc(easy_to_learn_candidates) do
    ratio_for_region =  $\min[samp\_ratio, \frac{n - |coreset|}{|region|}]$ 
    coreset.append(sample(region, ratio_for_region))
    remove region from easy_to_learn_candidates
    if  $|coreset| \geq n$  then return coreset
    end if
    if  $|easy\_to\_learn\_candidates| + |coreset| \leq n$  then
        Break
    end if
end for
add easy_to_learn_candidates to coreset
return coreset

```

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leaf in *leaves* contains any of the data points from that group. If such a leaf exists, we create a new group containing the common data points and add it to *new\_data\_groups*. After iterating through all the groups with respect to the leaves of the current tree, we obtain a collection of data groups characterized by varying levels of homogeneity concerning the label, different sizes, and diverse characteristics. We set this collection as the *data\_groups*. Subsequently, we review the groups within *data\_groups* and for either small groups (below the threshold) or homogeneous groups, we add them to *datamap* and remove them from *data\_groups*.

*Single Decision Tree Datamap creation.* To further accelerate our algorithm, we introduce a simplified approach for creating a datamap specifically tailored for a single decision tree. As demonstrated in Section 6, employing this method results in a runtime reduction of up to 75%, with only a slight decrease in the quality of the generated coreset.

## 4.2 Coreset Creation

Following the introduction of the datamap creation algorithm we present CoreTab (Algorithm 2), the algorithm responsible for selecting a coreset based on the user’s preferred coreset size.

*Initialization.* The algorithm begins by initializing an empty set for the coreset entity and executing Algorithm 1, which is the algorithm for GBDT datamap creation (explained in Section 4.1). Initially, all *hard* regions in the *datamap* are added to the *coreset*. These regions are defined as non-homogeneous regions formed in the datamap. If the required coreset size is reached, the algorithm stops and outputs the coreset. If the required size is not yet reached, the algorithm proceeds to add samples from the easy regions, starting with the largest *easy* regions. The set of candidates for *easy* regions is constructed initially by adding all homogeneous regions.

*Candidates Consideration.* An iterative process is then employed to determine the final composition of the coreset. The algorithm examines each region in the *easy* candidates, starting from the largest. For each region, the ratio at which this region will be sampled is defined as the minimum between the given *sample\_ratio* and the portion of the remaining space in the coreset needed to hold a sample of this region. The region is then sampled according to the defined sample ratio and added to the coreset, while being removed from the *easy* candidates. Taking a sample from a region enables the future ML model, trained solely on the coreset, to gain insight into this region, ensuring coverage even if not fully represented. This loop terminates either when the requested coreset size is reached or when all regions from the *easy* candidates are sampled. Because the candidates are sampled by the order of their size, we first take the *easy* regions and only then we get to the *amb* regions, if the current coreset size allows the addition of elements. This strategy (explained in more details in Section 3) is based on the observation that smaller groups are often harder for the algorithm to distinguish from examples of the other class, thus providing more valuable information for the training process.

*Performance and Explainability.* In Section 6, we present experimental results demonstrating the effectiveness of coresets generated by our proposed method compared to training models on the full dataset. These coresets consistently outperform all baseline approaches across various ML models, achieving performance levels closely aligned with models trained on the complete dataset. Additionally, the system offers a valuable explainability component by linking the coreset and the datamap, unveiling crucial patterns in the coreset, particularly those omitted, as detailed in Section 5.5. This feature enables users to evaluate the coreset’s suitability for their task and facilitates additional functionalities, including bias detection. Moreover, Section 5 introduces an algorithm for coreset creation that prioritizes optimization based on a user-defined quality metric, by leveraging an enhanced training method, capitalizing on the provided mathematical guarantees.

## 5 ENHANCING TRAINING FOR IMPROVED MODEL PERFORMANCE AND EXPLAINABILITY

Following coreset creation and ML model training, the inference phase involves presenting unseen data to predict labels. While training on our coreset yields performance akin to models trained on the full dataset (see Section 6), we introduce a novel method for further improvement. This approach provides mathematical guarantees for *multiple models* with a defined property, avoiding the usual restriction of guarantees to a single model. Users often explore various models before finding the most suitable one, making our method more relevant to real use-cases. To boost training outcomes, we advocate a departure from the conventional inference approach, and enhance predictions using the datamap. If a new data entry falls within *easy to learn* regions (not represented in the coreset), characterized by label homogeneity and straightforward classification, we predict the label associated with that datamap region, complementing the model’s output; otherwise, we rely solely on the model,

following standard inference based on the coreset-trained model. Efficient implementation is crucial, particularly with a large number of groups.\* In the remaining part of this section, we outline theoretical guarantees for our algorithm in the training enhancement context, first defining two types of errors when an ML model is solely trained on the coreset during inference. Note that although these definitions and guarantees are tailored for the binary classification scenario, a partial extension to multi-class classification is demonstrated in Section 6. Lastly, we introduce an additional algorithm to generate a coreset based on user-specified required performance, indicated by a quality metric. The promising experimental results are in Section 6.

### 5.1 Formal Definitions

In the context of our analysis, let’s consider a dataset  $D$  that can be partitioned into two subsets:  $P$  representing all the examples from the positive class and  $N$  representing all the examples from the negative class, formally,  $D = P \cup N$ . Next, let  $S, S' \subset D$ , denote the training and validation sets, respectively, randomly selected from  $D$ .

The datamap generation process (using Algorithm 1) operates on  $S$ , creating regions that are then classified into easy, ambiguous and hard to learn for the model. Then, Algorithm 2 creates the coreset, by focusing on the hard to learn regions, and the easy to learn regions are intentionally omitted or significantly under-represented by the coreset. This deliberate exclusion serves a dual purpose: it keeps the coreset small while enabling predictions for new entries during the inference phase based on the region to which they would be assigned in the datamap, particularly when these entries fall within the excluded easy to learn regions. These homogeneous regions are formally defined as follows:

Let  $p_1, \dots, p_{k_p} \subseteq D$  be the *easy to learn* and *ambiguous* regions in datamap that predominantly comprise positive examples, and formally, are positive homogeneous (given  $\psi$  homogeneity threshold):

$$\forall i, j \in [1, k_p] \quad \frac{|p_i \cap S \cap P|}{|p_i \cap S|} \geq \psi, \text{ \& \& } i \neq j \implies p_i \cap p_j = \emptyset,$$

Similarly,  $n_1, \dots, n_{k_n} \subseteq D$ , that primarily contain negative examples, are defined. The unions of these groups, and the complement sets are denoted as:

$$P' = \bigcup_{i=1}^{k_p} p_i, P'^c = \{x \in D \wedge x \notin P'\}, N' = \bigcup_{i=1}^{k_n} n_i, N'^c = \{x \in D \wedge x \notin N'\}$$

We now turn our attention to the two types of errors that can occur when an ML model is trained solely on the coreset, distinct from the entire dataset. To the best of our knowledge, this work is the first to provide theoretical guarantees for these types of errors.

*Errors on the Entries from the Coreset Distribution [CrsErr].* These errors occur when the model misclassified an unseen entry taken from the same distribution as the data points in the coreset. We determine if an entry belongs to the coreset distribution by examining the datamaps. An entry is considered part of the coreset distribution if it falls outside the regions in the datamap designated as *easy to learn* and thus intentionally excluded or significantly under-represented in the coreset. For simplicity, we assume that the sample ratio is 0. For this type of error, given that the examples falling within

\*To achieve this, we leverage the *Aho-Corasick* algorithm [8]. Utilizing a prefix tree structure, we concatenate the leaves of these groups, allowing for swift and accurate predictions during the inference phase, even when dealing with a substantial number of groups.

Data	Baselines	LR	SVM	XGB	LGBM	CAT	TABNET	RF
CC	CoreTabDT	<b>0.74±0.03</b>	<b>0.84 ± 0.02</b>	<b>0.87 ± 0.02</b>	0.84 ± 0.02	<b>0.87 ± 0.01</b>	0.1 ± 0.1	<b>0.86 ± 0.02</b>
	CoreTabGBT	0.73 ± 0.03	<b>0.84 ± 0.02</b>	<b>0.87 ± 0.02</b>	<b>0.86 ± 0.02</b>	<b>0.87 ± 0.02</b>	0.1 ± 0.1	0.85 ± 0.02
	Default	0.73 ± 0.04	0.78 ± 0.02	<b>0.87 ± 0.02</b>	0.83 ± 0.02	<b>0.87 ± 0.02</b>	<b>0.2 ± 0.2</b>	<b>0.86±0.02</b>
BF	CoreTabDT	<b>0.12±0.01</b>	0.088 ± 0.002	<b>0.192 ± 0.006</b>	0.103 ± 0.002	<b>0.216 ± 0.008</b>	0.083 ± 0.003	<b>0.14±0.01</b>
	CoreTabGBT	0.035 ± 0.004	<b>0.104 ± 0.002</b>	0.119 ± 0.007	<b>0.124 ± 0.003</b>	0.108 ± 0.005	<b>0.094±0.005</b>	0.018 ± 0.003
	Default	0.02 ± 0.003	N/A(24h+)	0.077 ± 0.006	0.096 ± 0.002	0.064 ± 0.005	0.081 ± 0.004	0.003 ± 0.001

**Figure 1: Performance (in terms of F1-Score) Comparison of Various ML Models Trained on Coresets Created by Two Versions of CoreTab and on the Entire Dataset (Default)**

the *easy to learn* regions, denoted as  $P'$  and  $N'$ , we define  $P' \cup N'$  as the union of all those regions. We denote  $(P' \cup N')^c$  as all the possible regions that do not intersect with  $(P' \cup N')$ . Consequently, we define the coreset as  $d = (P' \cup N')^c \cap S$ .

*Errors on the Entries from the Excluded Data Distribution [ExcErr].* This category of error materializes when the model makes a misclassification on an entry similar to the portions of the data that were deliberately excluded from the coreset. To determine if an entry is part of this excluded distribution, we rely on the datamaps, specifically checking whether it falls within the excluded regions. The model, having been trained on the coreset, has not encountered these data points during its training phase. Formally, if an entry falls within a region in  $P'$  ( $N'$ ), the probability that this entry belongs to the class  $N$  ( $P$ ) defines the likelihood of this type of error. Our inference method would predict that such an entry belongs to the positive (negative) class. We can formally define these probabilities as  $P(x \in P' | x \in N)$  and  $P(x \in N' | x \in P)$ , and by referring to  $x$  as Bernoulli variables, and  $S'$  as a sample of it, we can get an estimation of this probability:

$$N_p := \begin{cases} 1, & \text{if } x \in P', \text{ given } x \in N, \\ 0, & \text{otherwise, given } x \in N. \end{cases}, P_n := \begin{cases} 1, & \text{if } x \in N', \text{ given } x \in P, \\ 0, & \text{otherwise, given } x \in P. \end{cases}$$

We employ the concept of the *Confidence Interval for Bernoulli Variables*, specifically utilizing the *Wilson method* [43]. This method offers an improvement over the normal approximation interval, making it suitable for small samples and skewed observations. With it, we can compute an upper bound for both  $N_p$  and  $P_n$ . In this calculation, we make use of the validation set  $S'$  to estimate these probabilities and their respective boundaries. The Wilson confidence is used because we have just the validation set  $S'$  for the evaluation, but we would like to generalize the error for the whole distribution of the data  $D$ . Thus,  $S'$  is used to create an upper bound for  $P_n$ .

Note that confidence interval calculation methods necessitate a user-defined parameter, denoted as  $\delta$ , which signifies the desired confidence level for the variable to fall within the interval. This same  $\delta$  value is used to establish the precision and recall boundaries. Importantly, our empirical results consistently show a much higher success rate than the chosen  $\delta$  value. Therefore, when we refer to "by a probability of at least  $\delta$ ", we are indicating the upper bound of the probability associated with the *ExcErr* error. Formally:

$$\hat{P}_n = \text{WilsonCIUpperBound}(P \cap S', \delta) \geq P_n, P(x \in P' | x \in N) \leq \hat{N}_p$$

$$\hat{N}_p = \text{WilsonCIUpperBound}(N \cap S', \delta) \geq N_p, P(x \in N' | x \in P) \leq \hat{P}_n$$

**Precision and Recall.** The guaranteed boundaries presented in this section pertain to the model's precision and recall. Below is a brief overview of these crucial metrics including formal definitions.

*Precision.* Defined as the ratio of true positive predictions to the total number of positive predictions made by the model, and defined formally,

$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}} = P(x \in P_{pred} | x \in P)$$

*Recall.* Measures the proportion of actual positive instances that are correctly identified by the model. It answers the question, and defined formally,

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}} = P(x \in P | x \in P_{pred})$$

Where  $P_{pred}$  defined as the group of the positive predictions of the model. The probabilistic definitions are going to be helpful in the guaranties proof.

## 5.2 CrsErr Errors

Let us delve into the *CrsErr* errors, which are the errors on entries taken from the coreset distribution. As previously explained, we define an entry as taken from the coreset distribution when it does not fall within  $P' \cup N'$ . If a dataset and ML model hold the *Refined-fit* property, we claim that a model trained solely on the coreset  $d = (P' \cup N')^c \cap S$  will not be worse than a model trained on the entire set  $S$  when making predictions on entries taken from the coreset distribution. Expecting performance stability in the targeted regions during training is not only reasonable but echoes established methodologies, such as [37] emphasis on enhancing performance by focusing on *challenging to learn* examples. Similarly, [27] follows a comparable strategy by ignoring easily learnable examples through the *GOSS* sampling method.

*Intuition.* During the training of an ML model, the goal is to fit itself to the given data. As perfect fitting for all training data examples is often unattainable, a compromise is necessary to minimize overall loss. Intuitively, a model trained on specific regions, such as  $(P' \cap N')^c$ , is expected to outperform a model trained on a larger and more diverse set, like the entire training set  $S$ . This is because the former model can concentrate on fitting to the specific regions of interest, while the latter must generalize to a broader range of data. This becomes even more accurate when considering that the regions excluded from the coreset are presumed to be "easy" for an ML algorithm to learn. Formally,

**Refined-fit Property.** A model  $M$ , and a data subset  $B$ , satisfy the refined fit property if the model trained solely on a set  $B \cap S$ , where  $B \subseteq D$ , will not perform worse, in terms of classification performance (Precision and Recall), on a test set taken from the distribution of  $B \cap S'$  than the same model trained on the entire  $S$ .  $P_{pred}$  is the set of all the examples that the model  $M(S, conf, y)$  classified as class  $P$ .  $P_{pred}^*$  is the set of all the examples that the

model  $M(S \cap B, \text{conf}, y)$  classified as class  $P$ . And in equivalent formal statement:

$$\begin{aligned} P(x \in P_{pred} \cap B | x \in P) &\leq P(x \in P_{pred}^* \cap B | x \in P) \\ P(x \in P_{pred} \cap B | x \in N) &\geq P(x \in P_{pred}^* \cap B | x \in N) \end{aligned}$$

Justifying reliance on this property has a dual basis: it is easily verifiable with a given dataset and ML model, and its validation across 35 use-cases (5 datasets and 7 diverse ML models) in Section 6 establishes its common occurrence, making it practically applicable for guarantees. Moving forward, we will furnish guarantees for *ExcErr* errors, specifically addressing errors on entries from the excluded data distribution, provided they adhere to the property.

### 5.3 ExcErr Errors

Relying on our established property, we extend assurances to this error type, ensuring comprehensive performance guarantees for a model trained solely on the coreset. Below, we provide theoretical assurances regarding Recall and Precision, outlining the expected differences in these metrics between a model trained on the entire dataset and one trained solely on the coreset.

**Recall Guarantees.** We define the difference in the recall:

**PROPOSITION 5.1.** *If the Refined-fit property holds, the disparity in recall between a model trained on the entire dataset (recall) and the recall of a model trained on the coreset  $d$  (recall\*), with the addition of datamap utilization during inference, is governed by a probability denoted as  $\delta$ . This difference is bounded by  $\hat{P}_n$ , which represents the upper limit on the fraction of the intersection between all the positive class examples denoted as  $P$  and the negative easy to learn set  $N'$ . In mathematical terms:*

$$\text{recall} - \text{recall}^* = \Delta_{\text{recall}} \leq P(x \in N' | x \in P) = \hat{P}_n$$

**PROOF.** Given that  $P_{pred}$  is the set of all the examples that the model classified as class  $P$ , *recall* is defined as:  $\text{recall} = P(x \in P_{pred} | x \in P)$ . Next, we bound the *recall*\* as all the entries that we have predicted are from the positive class, put aside the entries that were part of  $N'$  and thus classified as false class, although their real classification is positive. Using the Refined-fit property:

$$\begin{aligned} \text{recall}^* &= P(x \in P_{pred}^* | x \in P) = P(x \in P_{pred}^* \cap (P' \cup N')^c | x \in P) \\ &+ P(x \in P_{pred}^* \cap (P' \cup N')^c | x \in P) \geq P(x \in P_{pred} \cap (P' \cup N')^c | x \in P) + P(x \in P' | x \in P) \\ &\geq P(x \in P_{pred} \cap (P' \cup N')^c | x \in P) + P(x \in P_{pred} \cap (P' \cup N') | x \in P) - P(x \in N' | x \in P) = \\ &= P(x \in P_{pred} | x \in P) - P(x \in N' | x \in P) \end{aligned}$$

Overall, the difference of the recall of the two models is:

$$\begin{aligned} \Delta_{\text{recall}} &= \text{recall} - \text{recall}^* \leq P(x \in P_{pred} | x \in P) - P(x \in P_{pred} | x \in P) \\ &+ P(x \in N' | x \in P) = P(x \in N' | x \in P) \end{aligned}$$

With  $\delta$  probability we get:  $\Delta_{\text{recall}} \leq P(x \in N' | x \in P) = \hat{P}_n$   $\square$

**Precision Guarantees.** We proceed to provide guarantees define the difference in precision:

**PROPOSITION 5.2.** *If the Refined-fit property holds, the difference in the precision of a model that was trained on all the data and the precision of the model that was trained on the coreset  $d$  and using the datamap in the inference, by probability of  $\delta$ , is:*

$$\hat{P}_n P(x \in P) + \frac{\hat{N}_p}{1 - P(x \in P)} + \hat{N}_p$$

This ratio highlights the connection between the percentage of the positive vs. negative, and  $\hat{N}_p, \hat{P}_n$  which represent errors of type *ExcErr* that our algorithm will make.

**PROOF.** We denote  $P_{pred}$  as all the examples that were classified as class  $P$  by the model. Thus, the precision of a model  $M$  trained over the whole training set  $S$  is:

$$\begin{aligned} \text{precision} &= P(x \in P | x \in P_{pred}) = \\ \frac{P(P \cap P_{pred})}{P_{pred}} &= \frac{P(P \cap P_{pred} \cap (P' \cup N')^c) + P(P \cap P_{pred} \cap P') + P(P \cap P_{pred} \cap N')}{P(P_{pred} \cap (P' \cup N')^c) + P(P_{pred} \cap P') + P(P_{pred} \cap N')} \end{aligned}$$

For brevity, we denote:

$$\gamma := +P(P \cap P_{pred}^c \cap P') + P(P_{pred} \cap N')$$

Now we will add the expression  $P(P \cap P_{pred}^c \cap P')$  to both the numerator and denominator, and as  $0 \leq \text{precision} \leq 1$ , the term will increase:

$$\begin{aligned} \text{precision} &\leq \\ &\leq \frac{P(P \cap P_{pred} \cap (P' \cup N')^c) + P(P \cap P_{pred} \cap P') + P(P \cap P_{pred}^c \cap P') + P(P \cap P_{pred} \cap N')}{P(P_{pred} \cap (P' \cup N')^c) + P(P_{pred} \cap P') + \gamma} = \\ &= \frac{P(P \cap P_{pred} \cap (P' \cup N')^c) + P(P \cap P') + P(P \cap P_{pred} \cap N')}{P(P_{pred} \cap (P' \cup N')^c) + (P(N \cap P_{pred} \cap P') + P(P \cap P_{pred} \cap P')) + \gamma} = \\ &= \frac{P(P \cap P_{pred} \cap (P' \cup N')^c) + P(P \cap P') + P(P \cap P_{pred} \cap N')}{P(P_{pred} \cap (P' \cup N')^c) + P(N \cap P_{pred} \cap P') + P(P \cap P') + P(P_{pred} \cap N')} = \\ &\leq \frac{P(P \cap P_{pred} \cap (P' \cup N')^c) + P(P \cap P') + P(P \cap P_{pred} \cap N')}{P(P_{pred} \cap (P' \cup N')^c) + P(P \cap P') + P(P_{pred} \cap N')} = \\ &= \frac{P(P \cap P_{pred} \cap (P' \cup N')^c) + P(P \cap P') + P(P \cap P_{pred} \cap N')}{(P(P \cap P_{pred} \cap (P' \cup N')^c) + P(N \cap P_{pred} \cap (P' \cup N')^c)) + P(P \cap P') + P(P_{pred} \cap N')} \leq \end{aligned}$$

Because the fraction is between 0 and 1, and using the refined-fit property, the same increase in both the numerator and denominator will increase the entire expression:

$$\leq \frac{P(P \cap P_{pred}^* \cap (P' \cup N')^c) + P(P \cap P') + P(P \cap P_{pred} \cap N')}{(P(P \cap P_{pred}^* \cap (P' \cup N')^c) + P(N \cap P_{pred} \cap (P' \cup N')^c)) + P(P \cap P') + P(P_{pred} \cap N')} \leq$$

Using the refined-fit property:

$$\begin{aligned} &\leq \frac{P(P \cap P_{pred}^* \cap (P' \cup N')^c) + P(P \cap P') + P(P \cap P_{pred} \cap N')}{(P(P \cap P_{pred}^* \cap (P' \cup N')^c) + P(N \cap P_{pred}^* \cap (P' \cup N')^c)) + P(P \cap P') + P(P_{pred} \cap N')} \leq \\ &\leq \frac{P(P \cap P_{pred}^* \cap (P' \cup N')^c) + P(P \cap P') + P(P \cap N')}{P(P_{pred}^* \cap (P' \cup N')^c) + P(P \cap P')} = \end{aligned}$$

Because  $P(P_{pred}^* \cap N') = 0$

$$= \frac{P(P \cap P_{pred}^* \cap P'^c) + P(P \cap P') + P(P \cap N')}{P(P_{pred}^* \cap P'^c) + P(P \cap P')} = \frac{B + P(P \cap N')}{A}$$

when  $1 \geq A \geq B$  and  $B \leq P(x \in P)$

Next we defined *precision\**, the precision achieved by a model that was trained on  $S$  without  $N'$ ,  $P'$  and in the inference phase, follows the training enhancement (the use of the datamap for predicting the labels of the entities that falls in the regions of  $N'$ ,  $P'$ ):

$$\begin{aligned} \text{precision}^* &= \frac{P(P \cap P_{pred}^* \cap P'^c) + P(P \cap P')}{P(P_{pred}^* \cap P'^c) + P(P_{pred}^* \cap P')} = \\ &= \frac{P(P \cap P_{pred}^* \cap P'^c) + P(P \cap P')}{P(P_{pred}^* \cap P'^c) + P(P \cap P') + P(x \in P' | x \in N)P(x \in N)} \end{aligned}$$

With probability  $\delta$  we get:

Baselines	CC			LN			CT			DI		
	F1-score	CCT (s)	MTT (s)	F1-score	CCT (s)	MTT (s)	F1-score	CCT (s)	MTT (s)	F1-score	CCT (s)	MTT
CoreTabDT	<b>0.87±0.02</b>	13.62 ± 1	0.35 ± 0.01	<b>0.985 ± 0.001</b>	92.5 ± 3	6.3 ± 0.3	0.793 ± 0.002	23.9 ± 0.5	0.64 ± 0.02	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
CoreTabGBT	<b>0.87±0.02</b>	6.8 ± 0.5	0.35 ± 0.01	<b>0.985 ± 0.001</b>	102 ± 1	6.3 ± 0.3	<b>0.849 ± 0.003</b>	85 ± 4	0.64 ± 0.02	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
TC	N/A	> 24h	N/A	N/A	> 24h	N/A	N/A	> 24h	N/A	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
CR	0.75 ± 0.05	10K ± 100	0.35 ± 0.01	N/A	OOM	N/A	0.839 ± 0.002	20K ± 1.6K	0.64 ± 0.02	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
SBT	0.80 ± 0.03	10.5K ± 200	0.35 ± 0.01	0.978 ± 0.001	48K ± 400	6.3 ± 0.3	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
RAN	0.79 ± 0.02	0.2 ± 0.01	0.35 ± 0.01	0.978 ± 0.001	0.1 ± 0.001	6.3 ± 0.3	0.835 ± 0.001	0.01 ± 0.02	0.64 ± 0.02	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
IS-CNN	0.50 ± 0.04	238 ± 10	0.35 ± 0.01	N/A	> 24	N/A	N/A	> 24	N/A	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
IS-CLUS	0.81 ± 0.01	719 ± 20	0.35 ± 0.01	0.94 ± 0.03	5K ± 70	6.3 ± 0.3	0.835 ± 0.003	830 ± 20	0.64 ± 0.02	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
FDMat	0.86 ± 0.017	0.7 ± 0.03	0.35 ± 0.01	0.97 ± 0.008	62 ± 3.21	6.3 ± 0.3	0.68 ± 0.009	2.02 ± 0.04	0.64 ± 0.02	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02
Default	<b>0.87±0.2</b>	N/A	7.1 ± 0.3	<b>0.985 ± 0.001</b>	N/A	165 ± 9	<b>0.849 ± 0.003</b>	N/A	6.6 ± 0.1	0.832 ± 0.002	11.4K ± 300	0.64 ± 0.02

**Figure 2: Baseline Comparison:** When the XGBoost model is trained on different coresets (including the entire dataset for the Default baseline), for various datasets (CC, LN, CT, DI), the coresets created by CoreTab outperform all other baselines in terms of F1-score. CoreTab also achieves significantly lower coreset creation times (CCT) compared to the more complex baselines. However, for a single run, it may sometimes take more time than training the default setting. This advantage becomes more apparent with repeated training. Model training time (MTT) remains consistent for all baselines that could create a coreset, except for the Default setting, which was trained on the entire dataset.

$$precision^* \geq \frac{P(P \cap P_{pred}^* \cap P^{rc}) + P(P \cap P')}{P(P_{pred}^* \cap P^{rc}) + P(P \cap P') + \hat{N}_p} = \frac{B}{A + \hat{N}_p} = \frac{1}{\frac{A}{B} + \frac{\hat{N}_p}{B}}$$

$$precision = \frac{B + P(x \in N' | x \in P)P(x \in P)}{A} \leq \frac{B + \hat{P}_n P(x \in P)}{A}$$

Thus, the difference between the precision of an ML model that has been trained over all  $S$  and the precision of a model that has been trained on a coreset  $d$  is:

$$\Delta_{precision} = precision - precision^* \leq \frac{\hat{P}_n P(x \in P)}{A} + \frac{1}{\frac{A}{B}} - \frac{1}{\frac{A}{B} + \frac{\hat{N}_p}{B}}$$

$$\hat{P}_n P(x \in P) + 1 - \frac{1}{1 + \frac{\hat{N}_p}{B}} \leq \hat{P}_n P(x \in P) + 1 - \frac{1}{1 + \frac{\hat{N}_p P(x \in N)}{P(x \in P) + \hat{N}_p P(x \in N)}}$$

$$= \hat{P}_n P(x \in P) + \frac{\hat{N}_p P(x \in N)}{P(x \in P) + \hat{N}_p P(x \in N)} = \hat{P}_n P(x \in P) + \frac{\hat{N}_p}{\frac{P(x \in P)}{P(x \in N)} + \hat{N}_p}$$

$$= \hat{P}_n P(x \in P) + \frac{\hat{N}_p}{\frac{1}{1 - \hat{P}(x \in P)} + \hat{N}_p}$$

□

**Further Discussion.** Note that specific algorithm performance (precision and recall) are not needed to calculate those boundaries, they are generic for all algorithms that satisfy the property. Also, it is crucial to highlight that there are no restrictions on the groups  $N'$  and  $P'$ , and the mathematical guarantees remain valid regardless of how they are selected. These guarantees naturally tend to improve when the groups exhibit higher homogeneity concerning the labels. Additionally, the coreset construction can be based on a subset of the features, not necessarily the entire feature set of the labeled data entries. Importantly, the mathematical guarantees provided above still hold in these scenarios. This flexibility allows the addition of features to an existing coreset during the feature engineering process while maintaining the mathematical guarantees. These claims have been proven in the experiments presented in Section 6.1.

## 5.4 opt\_per Algorithm

Now, having defined the mathematical guarantees for performance when the training enhancement approach is used, we present an algorithm for coreset creation that optimizes the coreset based on the quality metric provided by users. The algorithm is similar to Algorithm 2, with modifications for separating the *easy* regions into

mostly positive or negative homogeneous groups, as explained in this section. Algorithm 3, formally defined below, is designed to construct a coreset (*coreset*) from an original dataset ( $D$ ), divided into training and validation sets ( $S$  and  $S'$  respectively), ensuring high-quality performance metrics based on specified differences in recall and precision from an ML model trained on the entire data while holding the defined property. The process starts with the creation of a *datamap*, dividing the dataset into regions that capture relevant patterns. The algorithm then iterates through these regions, evaluating their homogeneity and ease of learning for positive and negative instances. Homogeneous regions are added to the coreset, with particular attention given to those conducive to learning positive and negative instances.

For negative instances, the algorithm selectively adds regions to the coreset until the desired recall threshold is met or exceeded. Sampling techniques maintain efficiency, and the selected regions are then removed from consideration. A similar process is applied to positive instances, ensuring the coreset achieves the specified precision threshold. This adaptive approach leverages validation sets and iterative adjustments to the coreset composition, dynamically accommodating different regions based on their learning complexities. The resulting coreset is a representative subset that optimally balances data inclusivity with computational efficiency, providing a valuable tool for subsequent machine learning tasks. The algorithm concludes by returning the generated coreset.

## 5.5 Explainability

This section concludes with an exploration of the explainability layer, which helps navigate the intricate trade-off between coreset size and recall or precision guarantees. We also provide insights into the resulting datamap, characterizing the selected coreset. We introduce a set of investigation tools to assist users in selecting the optimal coreset size for their specific needs and to gain deeper insights into the created coreset.

**Trade-off Visualization.** Unlike other approaches that either rely on default coreset size percentages or require user input, we offer users the ability to explore the impact of various coreset sizes on the model's *recall* and *precision*, guided by the mathematical guarantees outlined in Section 5. Figure 3 illustrates an example of an investigation trade-off graph generated for the *HP* dataset. This graph



**Algorithm 3** Creation of Datamap - Quality optimized

---

**Input:** Training set  $S \subset D$ , Validation set  $S' \subset D$ , recall threshold  $\tau_{recall}$  or precision threshold  $\tau_{precision}$ ,  $t_{num} = 30$ ,  $\tau = 5$ , sample ratio  $samp\_ratio$

**Output:**  $d = [r_{i_1}, r_{i_2}, \dots, r_{i_n}]$  coreset with performance  $\tau_{recall}$  or  $\tau_{precision}$

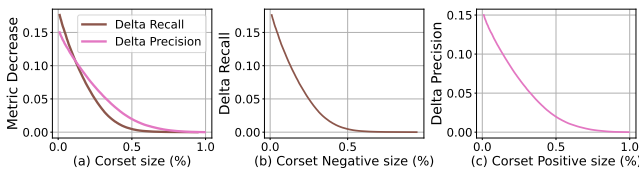
```

coreset = []
p_easy_to_learn_cand = []
n_easy_to_learn_cand = []
datamap = datamap_creation(S, tnum,  $\tau$ )
for region  $\in$  datamap do
    if homogeneous(region) = False then
        coreset.append(region  $\cap$  S)
    end if
    if homogeneous(region) = True & positive(region) = True then
        p_easy_to_learn_cand.append(region)
    end if
    if homogeneous(region) = True & negative(region) = True then
        n_easy_to_learn_cand.append(region)
    end if
end for
p_val = {}
n_val = {}
 $\Delta_{recall} = 0$ 
 $\Delta_{precision} = 0$ 
for region  $\in$  sort_by_size_desc(n_easy_to_learn_cand) do
    n_val.append(region  $\cap$  S')
     $\Delta_{recall} = calc\_delta\_recall(n\_val)$ 
    if  $\Delta_{recall} > \tau_{recall}$  then
        break
    end if
    coreset.append(sample(region  $\cap$  S, samp_ratio))
    remove region from n_easy_to_learn_cand
end for
add n_easy_to_learn_cand  $\cap$  S to coreset

for region  $\in$  sort_by_size_desc(p_easy_to_learn_cand) do
    p_val.append(region  $\cap$  S')
     $\Delta_{precision} = calc\_delta\_precision(p\_val, n\_val)$ 
    if  $\Delta_{precision} > \tau_{precision}$  then
        break
    end if
    coreset.append(sample(region  $\cap$  S, samp_ratio))
    remove region from p_easy_to_learn_cand
end for
add p_easy_to_learn_cand  $\cap$  S to coreset
return coreset
    
```

---

aids users in determining the most suitable coreset size for their task. Figure 3(a) showcases how *recall* and *precision* change when the coreset size varies, yet retains a stratified distribution of positive and negative examples. Furthermore, Figures 3(b) and (c) empower users to conduct deeper explorations into the effects of selecting different proportions of positive and negative examples, offering a high degree of flexibility in coreset customization through our algorithm.



**Figure 3: Trade-off: Coreset size vs Performance Guarantees (HP)**

**Coreset Explainability.** We further introduce a visualization tool designed to enhance user comprehension regarding the data patterns represented by regions in the datamap that were either omitted from

the coreset or included in a significantly reduced proportion due to their ease of learning by the algorithm. This visualization, presented as a decision tree, provides users with valuable insights into the entire dataset and its pertinent components for the specific classification tasks under examination.

## 6 EXPERIMENTS

Our system underwent thorough evaluation, assessing runtime performance and coreset quality with the F1-score metric across diverse models and datasets. We then evaluated the training enhancement method, including cross-validation testing, hyper-parameter tuning, and presenting empirical results for theoretical guarantees. Lastly, ablation studies are discussed.

**Experimental Setup.** Our system, implemented in Python 3.9 as a local library [1], is compatible with common EDA environments like Jupyter notebooks. We utilize the XGBoost library [2] for Gradient Boosting Decision Tree and scikit-learn [3] for the decision tree in the lighter version. The Aho-Corasick algorithm for inference uses the Python implementation [4]. Experiments ran on an Intel Xeon CPU server with 24 cores and 1024GB of RAM, using default parameters carefully tested, elaborated in this Section.

**Datasets** To demonstrate the versatility of our system, we used a variety of datasets with different characteristics, including balanced and unbalanced classes, varying sizes, and different combinations of column types (numeric, categorical, textual), all were previously used for coreset creation:

- (1) Credit Cards [3] (CC): 250K rows, 31 columns, 0.17% positive ( $P$ ) class.
- (2) Loans [6] (LN): 856K rows, 1145 columns, 5.4%  $P$  class.
- (3) Hempass [5] (HP): 7M rows, 29 columns, 50%  $P$  class.
- (4) Bank Fraud [1] (BF): 1M rows, 59 columns, 1.1%  $P$  class.
- (5) Diabetes [4] (DI): 254K rows, 22 columns, 14%  $P$  class.
- (6) Coverttype [2] (CT): 581K rows, 55 columns, 36%  $P$  class.

For brevity, results are presented for representative datasets in each experiment, showcasing diversity in class balance, column types, and size. Evaluation also includes a multi-class dataset (CT), utilizing the one-versus-all training method for the first class (class 1 in the dataset).

**Baselines.** In our comparative analysis, we evaluate various baseline methods for creating data samples or subsets and constructing tabular coresets tailored for model training. For all baselines, we imposed a limit on the coreset size of 30,000 examples per class. All baselines, extensively discussed in Section 2, include:

*Naive methods:*

- (1) RAN (*Random Sampling*): Randomly selects data tuples for forming a coreset.

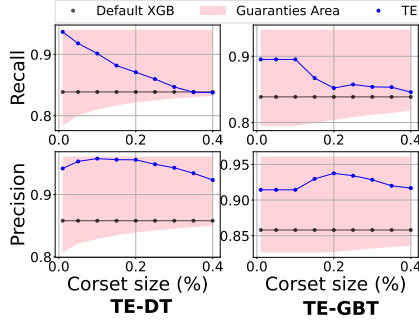
*Instance selection and Sampling Methods:*

- (2) IS-CNN (*Instance Selection - Condensed Nearest Neighbors*): Coreset selection for Condensed Nearest Neighbors classification [29], limited in adjusting coreset sizes.
- (3) IS-CLUS (*Instance Selection - Cluster Centroids*): Coreset selection using centroids of data clusters generated with a specified number of clusters [29].

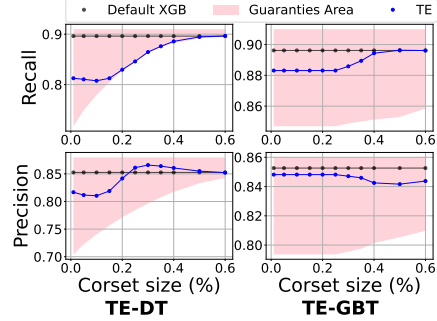
*Coresets selection methods:*

Baselines	CC (12%)			BF (6%)		
	F1-score 20%	F1-score 40%	F1-score 60%	F1-score 20%	F1-score 40%	F1-score 60%
CoreTabDT	<b>0.87±0.01</b>	<b>0.87±0.01</b>	0.86 ± 0.01	<b>0.187 ± 0.004</b>	<b>0.184 ± 0.004</b>	<b>0.185±0.003</b>
CoreTabGBT	<b>0.87±0.01</b>	<b>0.87±0.01</b>	0.86 ± 0.01	0.127 ± 0.005	0.121 ± 0.007	0.12 ± 0.01
TE-DT	<b>0.87±0.01</b>	0.86 ± 0.02	0.86 ± 0.02	0.121 ± 0.004	0.12 ± 0.01	0.10 ± 0.01
TE-GBT	<b>0.87±0.01</b>	<b>0.87±0.01</b>	0.86 ± 0.01	0.13 ± 0.01	0.124 ± 0.008	0.12 ± 0.01
Default	<b>0.87±0.01</b>	<b>0.87±0.01</b>	<b>0.87±0.01</b>	0.08 ± 0.01	0.08 ± 0.01	0.08 ± 0.01

**Figure 4: Robustness to Feature Addition:** The percentage indicates the portion of features remained in the training dataset. Even though CoreTab was trained on only a subset of the features, it selected rows representative of the entire dataset, resulting in model performance that either matched or exceeded that of the default model trained on the full dataset. This demonstrates CoreTab’s remarkable robustness to scenarios involving frequent feature addition.

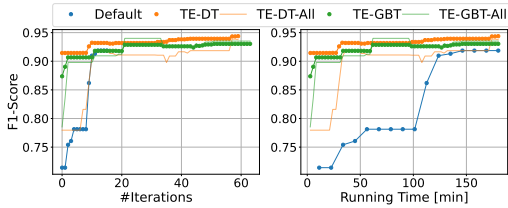


(a) Theoretical Guaranties Validation (CT)



(b) Theoretical Guaranties Validation (HP)

**Figure 5: Theoretical Guaranties Validation**



**Figure 6: Hyper-Parameters Optimization (CT)**

Model	Baselines	Default Recall	Corset Recall	Default Precision	Corset Precision
XGB	TE-DT	0.576 ± 0.012	0.69 ± 0.0126	0.653 ± 0.011	0.66 ± 0.008
	TE-GBT	0.696 ± 0.005	0.759 ± 0.009	0.669 ± 0.011	0.737 ± 0.012
LR	TE-DT	0.61 ± 0.003	0.645 ± 0.007	0.533 ± 0.009	0.528 ± 0.011
	TE-GBT	0.473 ± 0.016	0.48 ± 0.038	0.574 ± 0.013	0.573 ± 0.006

**Figure 7: Refined-fit property validation (CT)**

- (4) CR (*CRAIG*): Coresets optimized for Logistic Regression [32].
- (5) SBT (*SubStrat*): Genetic-based tuples selection for auto-ML training [28].
- (6) TC (*Tree Coreset*): Coresets for k decision trees [26].
- (7) FDMat (*FDMat*): The state-of-the-art coreset creation method for Computer Vision domain, adapted to tabular use-case [44].
- (8) CoreTab (*CoreTab*): Our implementation of Algorithm 2, with *CoreTab-GBT* using the GBDT datamap for coreset selection and *CoreTab-DT* using the datamap for a single Decision Tree. Both used sample ratio of 3%.

- (9) Default (*Default*) Training the algorithm on the entire dataset. While it is expected to outperform models trained on coreset, it requires significantly more time for training compared to models trained on a coreset alone.

**ML models tested** We test the created coreset over the performance of different ML models, all those models were used to train over the coreset that were created for different datasets, and by different baselines. We divide the tested models by type of ML model.

*Tree based:*

- (1) XGBoost [14] (XGB)
- (2) LightGBM [27] (LGBM)
- (3) CATboost [36] (CAT)
- (4) Random Forest [24] (RF)

*Classic ML:*

- (5) Logistic Regression [18] (LR)
- (6) Support Vector Machine (with RBF kernel) [17] (SVM).

*Neural Networks for tabular data:*

- (7) TabNet[9] (TABNET).

**Evaluation Metric** To assess the performance of classifiers trained on each coreset and the entire dataset, we use the *F1-score* for the positive class, which in unbalanced datasets is the smaller class. The F1-score is a crucial metric for evaluating classification models, especially in imbalanced datasets, as it considers both precision and recall, providing a balanced measure of model performance. This ensures that the model accurately identifies all classes. The F1-score is calculated using the harmonic mean of precision and recall, defined as follows:  $F1\text{-score} = 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$ , with precision and recall definitions provided in Section 5.

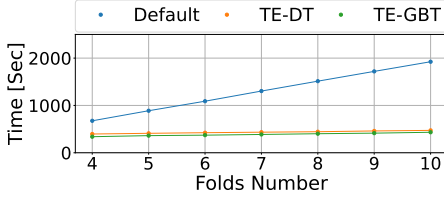


Figure 8: Cross Validation Running Time (LN)

## 6.1 CoreTab Evaluation

Next, we compare baseline performance using our quality metrics and execution time. The results are divided into two sections: baselines comparison and usability across different ML models. The experimental setup primarily prioritises optimising *opt\_size* as the main criterion. Given that the other baselines can only generate coresets of predetermined sizes, we included *opt\_size* experiments to ensure a fair comparison, as this is the standard task.

**Baseline Comparison.** Figure 2 presents the F1 scores for the XGBoost model when trained on coresets generated by various baselines. For each baseline and the datasets *CC*, *LN*, *CT*, and *DI*, we provide the F1 scores of models trained on the baselines’ coreset and the running times (in seconds). Across all four datasets, CoreTab consistently achieves the highest F1 scores (tied with *Default* that used the entire dataset). These scores are, on average, up to 10% higher than those of the other baselines. CoreTab also exhibits the second-best running times (excluding RAN), with coreset creation and model training typically completed in just a few minutes. Only FDMat had a faster runtime than ours; however, its performance was significantly worse. For instance, in the *CT* dataset, it produced the poorest F1-score. This demonstrates the effectiveness of our sampling algorithm in capturing relevant portions of large datasets with respect to their labels. Note that the direct competitor TC was unable to finish coreset creation within the reasonable time limit of 24 hours. Additionally, the CRAIG algorithm generates a similarity matrix between all data points during execution, resulting in a matrix size of 20TB for the *LN* dataset, exceeding the available memory, denoted as *OOM* (Out of Memory). Further comparisons involving the Logistic Regression model yield similar results, thus omitted.

**Performance over different ML models.** Figure 1 presents the performance of various ML models, both classic and complex, when trained on coresets generated by the two versions of CoreTab. These results are compared to the performance of the exact models and configurations trained on the entire dataset, rather than just the coreset. Notably, across all models and both datasets (*BF* and *CC*), CoreTab in both versions either performs on par with the default training on the full dataset or even outperforms it. Moreover, the lightweight version of our algorithm, CoreTabDT, exhibits nearly the same performance as the full version while significantly reducing computation time. In some cases, it even outperforms the full version. Notably, the SVM model did not complete training within 24 hours on the full *BF* and is thus absent from Figure 1. However, it successfully completed training on the coresets in less than an hour.

**Cross-Validation.** While a single run is significantly quicker than training the model on the entire dataset for some datasets, for others,

training over the whole dataset takes less time than creating the coreset and then training the model on it. However, the time saved using our coresets during cross-validation is noteworthy, as shown in Figure 8. For an XGBoost model on the *LN* dataset, even with a small number of folds, cross-validation takes nearly half the time when trained on the coreset. With an increasing number of folds, the time differences become more pronounced, resulting in only 25% of the runtime for a 10-fold cross-validation.

**Relevance of CoreTab to the Feature Addition Scenario.** In the context of working with tabular data, where it is common to gradually add features, our system’s robustness is a critical factor. To assess this, we conducted experiments focusing on the addition of features, particularly emphasizing the relevance of CoreTab in such scenarios. In the initial experiment, we deliberately excluded 20% – 60% of the columns from all datasets. Our coreset selection algorithm operated on this partial data, involving the creation of a datamap specifically tailored to the subset of features. Subsequently, we introduced the remaining columns to the coreset. Following this, an ML model was trained on the coreset, which was initially created with only a subset of the features. During the inference phase, the model was tested on the full test set, encompassing all features.

As illustrated in Figure 4, CoreTab exhibited remarkable performance. Even when created with only a subset of the features, it selected relevant tuples that effectively captured various aspects of the data. With the subsequent addition of features, these selected tuples retained their relevance for training an ML model. The performance of the ML model trained on this coreset not only outperformed models created by competitors but also matched the performance of a model trained on the entire dataset with all columns. To provide concrete examples, for the *CC* dataset, the performance of coresets selected using only part of the features (Figure 4) closely matched the performance of coresets selected using all features (Figure 2). Similarly, for the *BF* dataset, the performance was comparable to models trained on the entire dataset, not just the coreset.

## 6.2 Training Enhancement Contribution

Figure 10 evaluates the training enhancement method’s effectiveness throughout the training phase of four advanced algorithms trained on the CoreTab coreset, (Section 5). The performance is comparable to models trained on the entire dataset (*Default*) and even improves for most models. Examining a specific model, like XGBoost, reveals enhanced results with only a marginal increase in runtime. The coresets in this section are created with the same size limit mentioned in the experimental setup.

**Hyper-Parameters Optimization.** Next, we highlight the utility of training enhancement, extending beyond the fundamental training of a single algorithm. In Figure 6, we illustrate the hyperparameter optimization process for an XGBoost model on the *CT* dataset. The optimization is constrained to a 3-hour runtime. It’s important to note that XGBoost often requires extensive parameter tuning, and our optimization uses the Optuna algorithm. The F1-score, representing model performance, is measured on a fixed test set. This process was repeated and employed 5-fold cross-validation for result reliability. The results show that the optimization process on the coreset

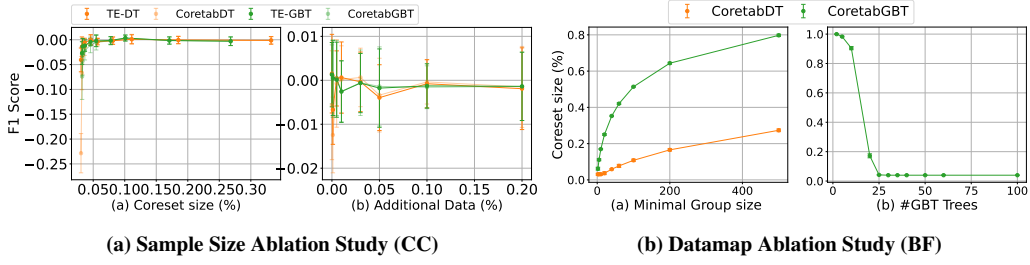


Figure 9: Ablation studies

Data	Baselines	XGB	LGBM	CAT	TABNET
CC (12%)	TE-DT	$0.87 \pm 0.02$	$0.86 \pm 0.02$	$0.87 \pm 0.01$	$0.3 \pm 0.1$
	TE-GBT	$0.87 \pm 0.02$	$0.86 \pm 0.02$	$0.87 \pm 0.02$	$0.3 \pm 0.1$
	Default	$0.87 \pm 0.02$	$0.83 \pm 0.02$	$0.87 \pm 0.02$	$0.2 \pm 0.2$
BF (6%)	TE-DT	$0.127 \pm 0.007$	$0.143 \pm 0.005$	$0.13 \pm 0.01$	$0.13 \pm 0.01$
	TE-GBT	$0.083 \pm 0.004$	$0.155 \pm 0.004$	$0.079 \pm 0.003$	$0.141 \pm 0.003$
	Default	$0.076 \pm 0.006$	$0.096 \pm 0.002$	$0.064 \pm 0.005$	$0.081 \pm 0.004$

**Figure 10: Training Enhancement Performance: ML models trained on the coresets generated by CoreTab, using the Training Enhancement method, achieve F1 scores that match or exceed those of the default setting where the model is trained on the entire dataset.**

outperforms the full dataset in terms of efficiency and time. Importantly, training the model with the optimized coreset configuration on the entire dataset yields excellent performance, highlighting the adaptability of coreset-generated configurations.

*Property Validation.* In Section 5, we introduced the mathematical guarantees of the training enhancement method, relying on the Refined-fit property of the model and data. This property has been thoroughly validated across various models and datasets, confirming its commonality and reliability. Figure 10 illustrates the validation of this property using the *CT* dataset, in conjunction with XGB and LR models. Notably, both versions of CoreTab either match or exceed the performance of the default algorithm trained on the entire dataset.

*Theoretical Guarantees Validation.* Next we provide empirical validation of the mathematical guarantees by Figure 5. The pink shaded region represents the guaranteed bounds for either the *recall* or *precision* results of the model trained on the coreset, for both versions of CoreTab, and for different coreset sizes. As shown, the performance of CoreTab consistently falls within the guaranteed bounds for all tested coreset sizes, often outperforming the default XGB model trained on the entire dataset. Note that the mathematical assurances for TE-GBT surpass those of TE-DT, this is TE-GBT main advantage over TE-DT.

### 6.3 Parameter Tuning and Ablation Studies

Here, we delve into the influence of critical parameters in our algorithm, which affect both coreset size and datamap creation.

*CoreTab Algorithm.* We conducted experiments to assess the influence of different parameters in the CoreTab algorithm by measuring the average F1-score achieved while varying one parameter and using default values for the others. The results, summarized in Figure 9a, highlight several key findings. Firstly, it is evident that the coreset should be at most 5% of the entire dataset, as increasing the

coreset size beyond this point does not significantly improve model performance. Additionally, we explored the impact of sampling from *easy-to-learn* regions and including them in the coreset. This parameter primarily affects when training enhancement method is not used. The experiments reveal that including more than 5% of entries from easy-to-learn regions in the coreset does not lead to substantial overall performance improvement.

*Datamap Algorithm.* We conducted experiments to assess the impact of different parameters in our datamap algorithm. By measuring the average coreset size achieved while varying individual parameters and keeping others at default values, we gained insights into their influence. Results, summarized in Figure 9b, indicated that increasing the minimum region size beyond 10 data entries notably expanded the coreset size, limiting data exclusion. Furthermore, varying the number of trees in the CoreTabGBT coreset creation phase showed minimal impact on coreset size, with inclusion of over approximately 30 trees yielding marginal changes.

## 7 CONCLUSION AND FUTURE WORK

In conclusion, we introduce CoreTab, an innovative algorithm designed for constructing data coresets optimized for training ML models using datamaps for GBDT models. Our experiments consistently showcase that these coresets, computed within minutes, surpass competing methods and even models trained on the full dataset. Moreover, a training enhancement technique leveraging datamap insights enhances performance with mathematical assurances, provided a defined property holds. Future research directions may include extending our method to handle multiple datasets, exploring its applicability to various model types, accommodating diverse data types including unstructured data, and adapting to multi-class classification.

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