AutoBalance: Optimized Loss Functions for Imbalanced Data

Anonymous Author(s)
Affiliation
Address
email

Abstract

Imbalanced datasets are commonplace in modern machine learning problems. The presence of under-represented classes or groups with sensitive attributes results in concerns about generalization and fairness. Such concerns are further exacerbated by the fact that large capacity deep nets can perfectly fit the training data and appear to achieve perfect accuracy and fairness during training, but perform poorly during test. To address these challenges, we propose AutoBalance, a bi-level optimization framework that automatically designs a training loss function to optimize a blend of accuracy and fairness-seeking objectives. Specifically, a lower-level problem trains the model weights, and an upper-level problem tunes the loss function by monitoring and optimizing the desired objective over the validation data. Our loss design enables personalized treatment for classes/groups by employing a parametric cross-entropy loss and individualized data augmentation schemes. We evaluate the benefits and transferability of our approach to the application scenarios of imbalanced and group-sensitive classification. Extensive empirical evaluations demonstrate the benefits of AutoBalance over state-of-the-art approaches. Our experimental findings are complemented with theoretical insights on loss function design and the benefits of the train-validation split.

1 Introduction

Recently, deep learning, large datasets, and the evolution of computing power have led to unprecedented success in computer vision, and natural language processing [15, 37, 58]. This success is partially driven by the availability of high-quality datasets, built by carefully collecting a sufficient number of samples for each class. In practice, real-world datasets are frequently imbalanced and exhibit long-tailed behavior, necessitating a careful treatment of the minorities [20, 50, 22]. Indeed, modern classification tasks can involve thousands of classes, so it is perhaps intuitive that some classes should be over/under-represented compared to others. Besides class imbalance, minorities can also appear at the feature-level; for instance, the specific values of the features of an example can vary depending on that example's membership in certain sensitive or protected groups, e.g. race, gender, disabilities (see also Figure 1a). In scenarios where imbalances are induced by heterogeneous client datasets (e.g., in the context of federated learning), addressing these imbalances can help ensure that a machine learning model works well for all clients, rather than just those that generate the majority of the training data. This rich set of applications motivate the careful treatment of imbalanced datasets.

In the imbalanced classification literature, the recurring theme is maximizing a fairness-seeking objective, such as balanced accuracy. Unlike standard accuracy, which can be dominated by the majorities, a fairness-seeking objective seeks to promote examples from minorities, and downweigh examples from majorities. Here, note that there is a distinction between the test and training objectives. While the overall goal is typically to maximize a non-differentiable objective such as balanced accuracy on the test set, during training, we use a differentiable proxy for this, such as

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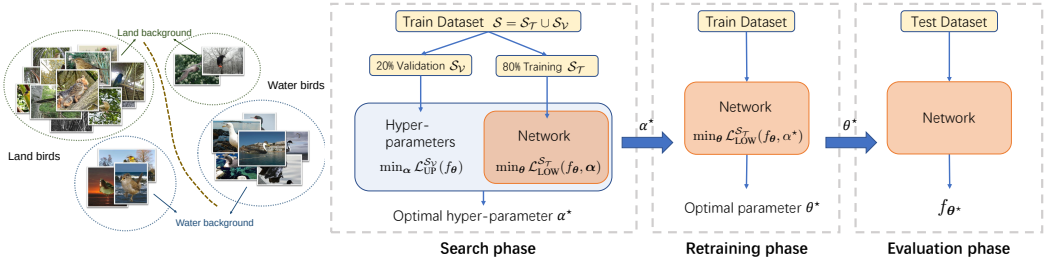


Figure 1: (a) Example group-imbalance on the Waterbirds dataset [59, 68]. Groups correspond to the distinct background types, while classes are distinct bird types. (b) Framework overview. The search phase conducts a bilevel optimization to design the optimal training loss function parameterized by $\boldsymbol{\alpha}^\star$ by minimizing the validation loss, using a train-validation split (e.g. 80%-20%). The retrain phase uses the original training data and $\boldsymbol{\alpha}^\star$ to obtain the optimal model parameters $\boldsymbol{\theta}^\star$. The evaluation phase predicts the test data using $\boldsymbol{\theta}^\star$.

weighted cross-entropy. Thus, the fundamental question of interest is:

How to design a training loss to maximize a fairness-seeking objective on the test set?

A classical answer to this question is to use a Bayes-consistent training loss function, so that as the sample size grows, the training process returns the Bayes-optimal decision rule. Thus, weighted cross-entropy (e.g., each class gets a different weight, see §4) is traditionally a good choice for optimizing weighted accuracy objectives. Unfortunately, this intuition starts to break down when the training problem is overparameterized, which is a common practice in deep learning: in essence, for large capacity deep nets, the training process can perfectly fit to the data, and training loss is no longer indicative of test error. In fact, recent works [8, 36] show that weighted cross-entropy has minimal benefit to balanced accuracy, and instead alternative methods based on margin adjustment can be effective (namely, by ensuring that minority classes are further away from decision boundary). These ideas led to the development of a parametric cross-entropy function $\ell(y, f(\boldsymbol{x})) = w_y \log\left(1 + \sum_{k \neq y} e^{l_k - l_y} \cdot e^{\Delta_k f_k(\boldsymbol{x}) - \Delta_y f_y(\boldsymbol{x})}\right)$, which allows for a personalized treatment of the individual classes via the design parameters $(w_k, l_k, \Delta_k)_{k=1}^K$ [8, 36, 50, 33, 63]. Here, w_k is the classical weighting term whereas l_k and Δ_k are additive and multiplicative logit adjustments. However, despite these developments, it is unclear how such parametric cross-entropy functions can be tuned for use for different fairness objectives, for example to tackle class or group imbalances. The works by [8, 50] provide theoretically-motivated choices for (w_k, l_k), while [36] argues that (w_k, l_k) is not as effective as Δ_k in the interpolating regime of zero training error. However, these works do not provide an optimized loss function that can be systematically tailored for different fairness objectives, such as balanced accuracy common in class imbalanced scenarios, or equal opportunity [22, 17] which is relevant in group-sensitive settings.

In this work, we address these shortcomings by designing the loss function within the optimization *in a principled fashion*, to handle different fairness-seeking objectives. Our main idea is to use bi-level optimization, where the model weights are optimized over the training data, and the loss function is automatically tuned by monitoring the validation loss. Our core intuition is that unlike training data, the validation data is difficult to fit and will provide a consistent estimator of the test objective.

Contributions. Based on this high-level idea, this paper takes a step towards a systematic treatment of imbalanced learning problems with contributions along several fronts: state-of-the-art performance, data augmentation, applications to different imbalance types, and theoretical intuitions. Specifically:

• We introduce *AutoBalance* —a bilevel optimization framework— that designs a fairness-seeking loss function by jointly training the model and the loss function hyperparameters in a systematic way (Figure 1b, Section 4). To further improve the test performance, our design also incorporates *data augmentation policies* personalized to subpopulations (classes or groups). We demonstrate the benefits of AutoBalance when optimizing various fairness-seeking objectives over the state-of-the-art, such as logit-adjustment (LA) [50] and label-distribution-aware margin (LDAM) [8] losses.

• Extensive experiments provide several takeaways (Section 5). First, the impact of individual design parameters in the loss function is revealed, with the additive adjustment l_k and multiplicative adjustment Δ_k synergistically improving the fairness objective. Second, personalized data augmentation

can further improve the performance over a single generic augmentation policy. Third, the loss functions designed by AutoBalance are transferable across datasets.

• Beyond class imbalance, we consider applications of loss function design to the group-sensitive setting (Section 6). Our experiments show that AutoBalance consistently outperforms various baselines, leading to a more efficient Pareto-frontier of accuracy-fairness tradeoffs.

2 Related Work

Our work relates to imbalanced classification, fairness, bilevel optimization, and data augmentation. Below we focus on the former three and defer the extended discussion to the supplementary.

Long-tailed learning. Learning with long-tailed data has received substantial interest historically, with classical methods focusing on designing sampling strategies, such as over- or under-sampling [38, 56, 9, 39, 1, 53, 64, 5, 47]. Several loss re-weighting schemes [51, 49, 24, 13, 6, 32] have been proposed to adjust weights of different classes or samples during training. Another line of work [66, 35, 50] focuses on post-hoc correction. More recently, several works [41, 33, 16, 32, 8, 13, 50, 63] develop more refined class-balanced loss functions (e.g. (4.1)) that better adapt to the training data. In addition, several works [28, 69] point out that separating the representation learning and class balancing can lead to improvements. In this work, our approach is in the vein of class-balanced losses; however, rather than fixing a balanced loss function (e.g. based on the class probabilities in the training dataset), we employ our Algorithm 1 to automatically guide the loss design.

Group-sensitive and Fair Learning. The group-sensitive learning aims to ensure the fairness of the classifier under setups where there exists under-represented groups (e.g., gender, race). [7, 22, 65, 60] propose several fairness metrics as well as insightful methodologies. A line of research [4, 19] optimize the worst-case loss over the test distribution and further applications motivate (label, group) metrics such as equality of opportunity [22, 17] (also recall DEO (3.1)). [54] discusses group-sensitive learning in an over-parameterized regime and proposes that strong regularization ensures fairness. Closer to our work, [54, 36] also study Waterbirds dataset. Compared to the regularization-based approach of [54], we explore a parametric loss design (which is inspired from [36]) to optimize fairness-risk over validation. [17] proposes methods and statistical guarantees for fair empirical risk minimization. A key observation of our work is that, such guarantees based on training-only optimization can be vacuous in the overparameterized regime. Thus, using train-validation split (e.g. our Algo 1) is critical for optimizing fairness metrics more reliably. This is verified by the effectiveness of our approach in the evaluations of Section 6.

Bilevel Optimization. Classical approaches [57] for hyper-parameter optimization are typically based on derivative-free schemes, including random search [61] and reinforcement learning [71, 3, 62, 67]. Recently, a growing line of works focus on differentiable algorithms that are often faster and can scale up to millions of parameters [43, 46, 55, 26, 45]. These techniques [42, 34, 70, 44] with continuous relaxations have shown significant success in neural architecture search, learning rate scheduling, regularization, etc. These methods are typically formulated as a bilevel optimization problem: the upper and lower optimizations minimize the validation and training losses, respectively. Some theoretical guarantees (albeit restrictive) are also available [11, 21, 2, 52]. Different from these, our work focuses on principled design of training loss function to optimize fairness-seeking objectives for imbalanced data. Here, a key algorithmic distinction (e.g. compared to architecture search) is that, our loss function design is only used during optimization and not during inference. This leads to a more sophisticated hyper-gradient and necessitates additional measures to ensure stability of our approach (see Algo 1).

3 Problem Setup

Let $[K]$ denote the set $\{1, \ldots, K\}$. Let 1_E be the indicator function of event E. Suppose we have a dataset $\mathcal{S} = (\boldsymbol{x}_i, y_i, g_i)_{i=1}^n$ sampled i.i.d. from a distribution $\mathcal{D}$ with input space $\mathcal{X}$, K classes and G groups. For an example $(\boldsymbol{x}, y, g)$, $\boldsymbol{x} \in \mathcal{X}$ is the input features, $y \in [K]$ is the output label, and $g \in [G]$ is the group membership. Let $f : \mathcal{X} \to \mathrm{R}^K$ be a model that outputs a distribution over classes and let $\hat{y}_f(\boldsymbol{x}) = \arg\max_{i \in [K]} f(\boldsymbol{x})$. Standard classification error is defined as $\mathcal{E}(f) = \mathrm{P}_{\mathcal{D}}[y \neq \hat{y}_f(\boldsymbol{x})]$. Let $\ell(y, \hat{y})$ be a differentiable proxy for 0-1 loss (specifically cross-entropy). We similarly denote

$$\text{Population risk: } \mathcal{L}(f) = \mathrm{E}_{\mathcal{D}}[\ell(y, \hat{y}_f(\boldsymbol{x}))], \quad \text{Empirical risk: } \mathcal{L}^{\mathcal{S}}(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, \hat{y}_f(\boldsymbol{x}_i)).$$

Algorithm 1: Bilevel Optimization for AutoBalance

Input: Model $f_{\boldsymbol{\theta}}$ with weights $\boldsymbol{\theta}$, dataset $\mathcal{S} = \mathcal{S}_{\mathcal{T}} \cup \mathcal{S}_{\mathcal{V}}$, step sizes $\eta_{\boldsymbol{\alpha}}$ & $\eta_{\boldsymbol{\theta}}$, # iterations $t_2 > t_1$

Initialize $\boldsymbol{\alpha}$ with $\ell_{\text{UP}}(\cdot) = \ell_{\text{LOW}}(\cdot; \boldsymbol{\alpha})$ `// Consistent initialization`

Train $\boldsymbol{\theta}$ for t_1 iterations ($\boldsymbol{\alpha}$ is fixed) `// Warm-up training`

for $i \leftarrow t_1$ **to** t_2 **do**

  Sample training batch $\mathcal{B}_{\mathcal{T}}$ from $\mathcal{S}_{\mathcal{T}}$;

  `// Apply class-personalized augmentation` $\mathcal{B}_{\mathcal{T}} \leftarrow \mathcal{A}(\mathcal{B}_{\mathcal{T}})$ `(implicitly)`

  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta_{\boldsymbol{\theta}} \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\text{LOW}}^{\mathcal{B}_{\mathcal{T}}}(f_{\boldsymbol{\theta}}; \boldsymbol{\alpha})$

  Sample validation batch $\mathcal{B}_{\mathcal{V}}$ from $\mathcal{S}_{\mathcal{V}}$;

  Compute hyper-gradient $\nabla_{\boldsymbol{\alpha}} \mathcal{L}_{\text{UP}}^{\mathcal{B}_{\mathcal{V}}}(f_{\boldsymbol{\theta}})$ `//via Implicit Differentiation e.g. [43]`

  $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha} - \eta_{\boldsymbol{\alpha}} \nabla \mathcal{L}_{\text{UP}}^{\mathcal{B}_{\mathcal{V}}}(f_{\boldsymbol{\theta}})$ `//Update loss function hyper-parameters`

end

Set $\boldsymbol{\alpha}_\star \leftarrow \boldsymbol{\alpha}$, $\mathcal{S}_{\mathcal{T}} \leftarrow \mathcal{S}$, reset weights $\boldsymbol{\theta}$

Train $\boldsymbol{\theta}$ for t_2 iterations using $\boldsymbol{\alpha}_\star$ `// Final training over full` $\mathcal{S}$ `using` $\boldsymbol{\alpha}_\star$

Result: The final model $\boldsymbol{\theta}_\star \leftarrow \boldsymbol{\theta}$ and hyper-parameters $\boldsymbol{\alpha}_\star$

For $(\boldsymbol{x}, y, g) \sim \mathcal{D}$, define the class, group, and (class, group) frequencies as follows

$$\boldsymbol{\pi}_k = \mathrm{P}_{\mathcal{D}}(y = k), \quad \bar{\boldsymbol{\pi}}_j = \mathrm{P}_{\mathcal{D}}(g = j), \quad \text{and} \quad \boldsymbol{\pi}_{k,j} = \mathrm{P}_{\mathcal{D}}(y = k, g = j), \quad \text{for} \quad (k, j) \in [K] \times [G].$$

Similarly, given sample $(\boldsymbol{x}, y, g)$ from $\mathcal{D}$, let $\mathcal{D}_k$ be the distribution conditioned on class $y = k$, let $\bar{\mathcal{D}}_j$ be the distribution conditioned on group $g = j$, let $\mathcal{D}_{k,j}$ be the distribution of $(\boldsymbol{x}, y, g)$ conditioned on $y = k$ and $g = j$. We say that a problem has class (or group) imbalance if majority class (or group) is substantially more frequent than minority. We introduce

$$\text{Class-conditional risk: } \mathcal{L}_k(f) = \mathrm{E}_{\mathcal{D}_k}[\ell(y, \hat{y}_f(\boldsymbol{x}))], \quad \text{Balanced risk: } \mathcal{L}_{\text{bal}}(f) = \frac{1}{K} \sum_{k=1}^{K} \mathcal{L}_k(f).$$

Similarly, group and (class, group)-conditional risks are denoted via $\bar{\mathcal{L}}_j(f)$ and $\mathcal{L}_{k,j}(f)$ respectively. We restrict our attention to the following applications that can benefit from our approach.

✓ **Setting A: Imbalanced classes.** This occurs when class frequencies differ, i.e., $\max_{i \in [K]} \boldsymbol{\pi}_i \gg \min_{i \in [K]} \boldsymbol{\pi}_i$. In this setting, we ignore group membership and focus on classes. Instead of standard accuracy, we will optimize a class-balanced error $\mathcal{E}_{\text{bal}}(f)$ by designing a class-personalized loss.

✓ **Setting B: Imbalanced groups.** This occurs when group or (class, group) frequencies differ, i.e., $\max_{j \in [G]} \bar{\boldsymbol{\pi}}_j \gg \min_{j \in [G]} \bar{\boldsymbol{\pi}}_j$ or $\max_{(k,j)} \boldsymbol{\pi}_{k,j} \gg \min_{(k,j)} \boldsymbol{\pi}_{k,j}$. Specifically, in the fairness literature, groups represent sensitive or protected attributes. A typical goal is ensuring that the prediction of the model is independent of these attributes. While many fairness metrics exist, in this work, we focus on the Difference of Equal Opportunity (DEO) [22, 17]. Our evaluations also focus on binary classification (with labels denoted via $\pm$) and two groups ($K = G = 2$). With this setup, the DEO risk is defined as $\mathcal{L}_{\text{DEO}}(f) = |\mathcal{L}_{+,1}(f) - \mathcal{L}_{+,2}(f)|$. When both classes are equally relevant (rather than $y = +1$ implying a semantically positive outcome), we use the following definition:

$$\mathcal{L}_{\text{DEO}}(f) = |\mathcal{L}_{+,1}(f) - \mathcal{L}_{+,2}(f)| + |\mathcal{L}_{-,1}(f) - \mathcal{L}_{-,2}(f)|. \tag{3.1}$$

4 Loss Function Design and Proposed Method

Our main goal in this paper is automatically designing loss functions to optimize target objectives for imbalanced learning (e.g., Settings A and B). We will employ a parametrizable family of loss functions that can be tailored to the needs of different classes or groups. Cross-entropy variations have been proposed by [41, 33, 16] to optimize balanced objectives. Our design space will utilize recent works by [36, 63], who introduce Vector Scaling (VS)-loss and Class-Dependent Temperatures (CDT). Specifically, for Setting A[1] we build on the following loss function parametrized by three vectors $\boldsymbol{w}, \boldsymbol{l}, \boldsymbol{\Delta} \in \mathrm{R}^K$:

$$\ell(y, f(\boldsymbol{x})) = w_y \log \left(1 + \sum_{k \neq y} e^{l_k - l_y} \cdot e^{\Delta_k f_k(\boldsymbol{x}) - \Delta_y f_y(\boldsymbol{x})} \right). \tag{4.1}$$

[1]Discussion of Setting B (group-imbalance) is deferred to Section 6, however the main ideas are similar.

This loss is same as VS-loss of [36], which also contains $\boldsymbol{w}, \boldsymbol{l}, \boldsymbol{\Delta} \in \mathrm{R}^K$. However, the denominator of VS-loss uses Δ_y whereas we use Δ_k similar to CDT of [63]. Here, w_y enables conventional weighted CE and l_y is the additive adjustment to the logits. Recently [50] proposed a Fisher consistent logit adjustment (LA) loss parameterized by w_y and l_y; we make the following related observation.

Lemma 1 *Parametric loss function* (4.1) *is not consistent for standard or balanced errors if there are distinct multiplicative adjustments i.e.* $\Delta_i \neq \Delta_j$ *for some* $i, j \in [K]$.

While consistency is a desirable property, it is intuitively more critical during the earlier phase of the training where the training risk is more indicative of the test risk. In the interpolating regime of zero-training error, [36] shows that $\boldsymbol{w}, \boldsymbol{l}$ can be ineffective and multiplicative $\boldsymbol{\Delta}$-adjustment can be more favorable. Our algorithm will be initialized with a consistent weighted-CE; however, we will allow the algorithm to automatically adapt to the interpolating regime by tuning $\boldsymbol{l}$ and $\boldsymbol{\Delta}$.

Proposed training loss function. For our algorithm, we will augment (4.1) with *data augmentation* that can be *personalized to distinct classes*. Let us denote the data augmentation policies by $\mathcal{A} = (\mathcal{A}_y)_{y=1}^K$ where each $\mathcal{A}_y$ stochastically augments an input example with label y. Additionally, we clamp $\boldsymbol{\Delta}_i$ with the sigmoid function σ to limit its range to (0,1) to ensure non-negativity. To this end, our loss function for the lower-level optimization (over training data) is as follows:

$$\ell_{\text{LOW}}(y, \boldsymbol{x}, f; \boldsymbol{\alpha}) = -\,\mathrm{E}_{\mathcal{A}}\left[w_y \log\left(\frac{e^{\sigma(\Delta_y) f_y(\mathcal{A}_y(\boldsymbol{x})) + l_y}}{\sum_{i\in[K]} e^{\sigma(\Delta_i) f_i(\mathcal{A}_y(\boldsymbol{x})) + l_i}} \right) \right]. \tag{4.2}$$

Here, $\boldsymbol{\alpha}$ is the set of hyperparameters of the loss function that we wish to optimize, specifically $\boldsymbol{\alpha} = [\boldsymbol{w}, \boldsymbol{l}, \boldsymbol{\Delta}, \text{param}(\mathcal{A})]$. param$(\mathcal{A})$ is the parameterization of the augmentation policies $(\mathcal{A}_y)_{y\in[K]}$.

Personalized data augmentation (PDA). Remarkable benefits of data augmentation techniques provide a natural motivation to investigate whether one can benefit from learning class-personalized augmentation policies. To explain our intuition, consider a spherical augmentation strategy where $\mathcal{A}_y(\boldsymbol{x})$ samples a vector uniformly from an ℓ_2-ball of radius ε_y around $\boldsymbol{x}$. As visualized in Figure 2 for a linear classifier, if the augmentation strengths of both classes are equal, the max-margin classifier is not affected by the application of the data augmentation and remains identical. Thus, augmentation has no benefit. However by applying a stronger augmentation on minority, the decision boundary is shifted to protect minority which can provably benefit the balanced accuracy [36, 8]. The following intuitive observation links the PDA to parametric loss (4.1).

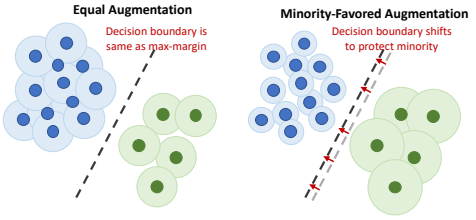


Figure 2: Data augmentation can shift the decision boundary to benefit the minority class by providing a larger margin. Lemma 2 establishes an equivalence between spherical data augmentation and parametric cross-entropy loss.

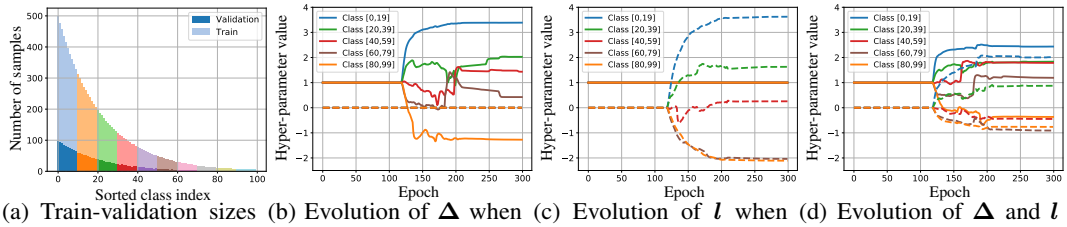
Lemma 2 *Consider a binary classification task with labels* 0 *and* 1 *and a linearly separable training dataset. For any parametric loss* (4.1) *choices of* $(l_i, \Delta_i, w_i)_{i=0}^1$*, there exists spherical augmentation strengths for minority/majority classes so that, without regularization,* ***optimizing the logistic loss with personalized augmentations returns the same classifier as optimizing*** (4.1)**.**

This Lemma is similar in flavor to the result of [29], which considers a larger uncertainty set around the minority class. As discussed in the supplementary materials, Lemma 2 is relevant for the overparameterized regime whereas the approach of [29] is ineffective for separable data [48]. Algorithmically, the augmentations that we consider are much more flexible than the ℓ_p-balls of [29] and our experiments showcase the value of our approach in state-of-the-art multiclass settings. Finally, we note that, the (theoretical) benefits of PDA can go well-beyond Lemma 2 by leveraging the invariances [10, 14] (via rotation, translation).

4.1 Proposed Bilevel Optimization Method

We formulate the loss function design as a bilevel optimization over $\boldsymbol{\alpha}$ and a hypothesis set $\mathcal{F}$. Split the dataset $\mathcal{S}$ into training $\mathcal{S}_{\mathcal{T}}$ and validation $\mathcal{S}_{\mathcal{V}}$ sets with $n_{\mathcal{T}}$ and $n_{\mathcal{V}}$ examples respectively. The upper-level variable $\boldsymbol{\alpha}$ aims to minimize a desired fairness-seeking objective $\ell_{\text{UP}}(y, \hat{y})$, and the lower-level hypothesis $f \in \mathcal{F}$ aims to minimize the training loss (4.2) as follows:

$$\min_{\boldsymbol{\alpha}} \mathcal{L}_{\text{UP}}^{\mathcal{S}_{\mathcal{V}}}(f_{\boldsymbol{\alpha}}) \quad \text{WHERE} \quad f_{\boldsymbol{\alpha}} = \arg\min_{f\in\mathcal{F}} \mathcal{L}_{\text{LOW}}^{\mathcal{S}_{\mathcal{T}}}(f; \boldsymbol{\alpha}) := \frac{1}{n_{\mathcal{T}}} \sum_{i=1}^{n_{\mathcal{T}}} \ell_{\text{LOW}}(y_i, \boldsymbol{x}_i, f; \boldsymbol{\alpha}). \tag{4.3}$$



(a) Train-validation sizes for CIFAR-100-LT clusters (b) Evolution of $\boldsymbol{\Delta}$ when only training $\boldsymbol{\Delta}$ (c) Evolution of $\boldsymbol{l}$ when only training $\boldsymbol{l}$ (d) Evolution of $\boldsymbol{\Delta}$ and $\boldsymbol{l}$ when optimizing jointly

Figure 3: (a) Visualizing class clustering and train-validation split. (b), (c), (d) Evolution of loss function parameters $\boldsymbol{l}, \boldsymbol{\Delta}$ over epochs for CIFAR-100-LT where solid curves and dashed curves corresponds to $\boldsymbol{\Delta}$ and $\boldsymbol{l}$ respectively. We display average value of 20 classes for better visualization

Here, $\mathcal{L}_{\text{UP}}$ is obtained as the empirical average of ℓ_{UP}. The function ℓ_{UP} is weighted cross-entropy, chosen to be a consistent proxy for the desired accuracy objective $\mathcal{E}_{\text{UP}}$. For instance, if $\mathcal{E}_{\text{UP}}$ is a superposition of standard and balanced errors $\mathcal{E}_{\text{UP}} = (1-\lambda)\mathcal{E} + \lambda\mathcal{E}_{\text{bal}}$, then similarly $\mathcal{L}_{\text{UP}} = (1-\lambda)\mathcal{L} + \lambda\mathcal{L}_{\text{bal}}$. Algorithm 1 summarizes our approach and highlights the key components. The training loss $\ell_{\text{LOW}}(\cdot;\boldsymbol{\alpha})$ is also initialized as a consistent proxy for $\mathcal{E}_{\text{UP}}$ (e.g. same as ℓ_{UP}).

Implicit Differentiation and Warm-up training. For a loss function parameter $\boldsymbol{\alpha}$, the hyper-gradient can be written via the chain-rule $\frac{\partial \mathcal{L}_{\text{UP}}(\boldsymbol{\theta}^\star)}{\partial \boldsymbol{\alpha}} = \frac{\partial \mathcal{L}_{\text{UP}}(\boldsymbol{\theta}^\star)}{\partial \boldsymbol{\theta}^\star}\frac{\partial \boldsymbol{\theta}^\star}{\partial \boldsymbol{\alpha}}$ Here, $\boldsymbol{\theta}^\star$ is the solution of the lower-level problem. We note that $\partial\mathcal{L}_{\text{UP}}/\partial\boldsymbol{\alpha} = 0$ since $\boldsymbol{\alpha}$ does not appear within the upper-level loss. Also observe that $\partial\mathcal{L}_{\text{UP}}(\boldsymbol{\theta}^\star)/\partial\boldsymbol{\theta}^\star$ can be directly computed by taking the gradient. To compute $\partial\boldsymbol{\theta}^\star/\partial\boldsymbol{\alpha}$, we follow the recent work by [43] and employ the Implicit Function Theorem (IFT). If there exists a fixed point $(\boldsymbol{\theta}^\star,\boldsymbol{\alpha}^\star)$ that satisfies $\partial\mathcal{L}_{\text{LOW}}(\boldsymbol{\theta}^\star,\boldsymbol{\alpha}^\star)/\partial\boldsymbol{\theta} = 0$ and regularity conditions are satisfied, then around $\boldsymbol{\alpha}^\star$, there exists a function $\boldsymbol{\theta}(\boldsymbol{\alpha})$ such that $\boldsymbol{\theta}(\boldsymbol{\alpha}^\star) = \boldsymbol{\theta}^\star$ and we also have $\frac{\partial\boldsymbol{\theta}}{\partial\boldsymbol{\alpha}} = (\frac{\partial^2\mathcal{L}_{\text{LOW}}}{\partial\boldsymbol{\theta}^2})^{-1}\frac{\partial^2\mathcal{L}_{\text{LOW}}}{\partial\boldsymbol{\theta}\partial\boldsymbol{\alpha}}$. However, directly computing inverse Hessian $(\frac{\partial^2\mathcal{L}_{\text{LOW}}}{\partial\boldsymbol{\theta}^2})^{-1}$ is usually time consuming or even impossible for modern neural networks which have millions of parameters. To compute the hyper-gradient while avoiding extensive computation, we approximate the inverse Hessian via the Neumann series, which is widely used for inverse Hessian estimation [40, 43]. Finally, the warm-up phase of our method (Line 2 of Algo. 1) is essential to guarantee that the IFT assumption $\frac{\partial\mathcal{L}_{\text{LOW}}(\boldsymbol{\theta}^\star,\boldsymbol{\alpha}^\star)}{\partial\boldsymbol{\theta}} = 0$ is approximately satisfied.

Why is train-validation split critical? It is well-understood that large capacity neural networks can perfectly fit and achieve 100% training accuracy [18, 72, 27]. This also implies that over the training data, different accuracy metrics or fairness constraints can be perfectly satisfied (e.g. 100% balanced accuracy, and 0% DEO). To truly find a model that lies on the Pareto-front of the (accuracy, fairness) tradeoff, the optimization procedure should (approximately) evaluate on the population loss. To this end, the validation phase provides this crucial population loss-proxy in the overparameterized setting where training error can be vacuous. Following the literature [30, 31], the intuition is that, as the dimensionality of the hyper-parameter $\boldsymbol{\alpha}$ is typically smaller than the validation size $n_{\mathcal{V}}$, validation loss will not overfit and will be indicative of the test even if the training loss is zero. In the supplementary materials, we formalize this intuition with emphasis on multi-objective tradeoffs; namely, under intuitive stability conditions, we show that a small amount of validation data is sufficient to ensure that the Pareto-front of the validation risk uniformly approximates that of the test-risk. Concretely, for two objectives $(\mathcal{L}_1, \mathcal{L}_2)$, uniformly over all λ, the $\boldsymbol{\alpha}$ minimizing the validation risk $\mathcal{L}_{\text{UP}}^{\mathcal{S}_{\mathcal{V}}}(f) = (1-\lambda)\mathcal{L}_1^{\mathcal{S}_{\mathcal{V}}} + \lambda\mathcal{L}_2^{\mathcal{S}_{\mathcal{V}}}$ in (4.3) also approximately minimizes the test risk $\mathcal{L}_{\text{UP}}(f)$.

5 Evaluations for Imbalanced Classes

In this section, we present our experiments on various datasets (CIFAR-10, CIFAR-100, iNaturalist-2018 and ImageNet) when the classes are imbalanced. The goal is to understand whether our bilevel optimization can design effective loss functions that improve balanced error $\mathcal{E}_{\text{bal}}$ on the test set. The setup is as follows. $\mathcal{E}_{\text{bal}}$ is the test objective. The validation loss $\mathcal{L}_{\text{UP}}$ is the balanced cross-entropy CE_{bal}. We consider various designs for ℓ_{LOW} such as individually tuning $\boldsymbol{w}, \boldsymbol{l}, \boldsymbol{\Delta}$ and augmentation. We report the average result of 3 random experiments under this setup.

Datasets. We follow previous works [50, 13, 8] to construct long-tailed versions of the datasets. Specifically, for a K-class dataset, we create a long-tailed dataset by reducing the number of

Method	CIFAR-10-LT	CIFAR100-LT	ImageNet-LT	iNaturalist
Cross-Entropy	30.33	62.69	60.81	39.76
LDAM loss [8]	26.45	59.40	58.14	35.42
LA loss ($\tau = 1$) [50]	23.32	58.92	55.60	34.37
Algo. 1: $\boldsymbol{\alpha} \leftarrow \tau$ of LA loss	21.75	58.76	55.16	34.18
Algo. 1: $\boldsymbol{\alpha} \leftarrow \boldsymbol{l}$	22.86	58.73	55.39	34.42
Algo. 1: $\boldsymbol{\alpha} \leftarrow \boldsymbol{\Delta}$	22.52	58.49	54.72	34.14
Algo. 1: $\boldsymbol{\alpha} \leftarrow \boldsymbol{\Delta}\&\boldsymbol{l}$	21.39	56.77	52.90	33.16
Algo. 1: $\boldsymbol{\alpha} \leftarrow \boldsymbol{\Delta}\&\boldsymbol{l}$, LA init	**21.16**	**56.71**	**51.96**	**33.09**

Table 1: Evaluations of balanced accuracy on long-tailed data. Algo. 1 with $\boldsymbol{\Delta}\&\boldsymbol{l}$ design space and LA initialization (bottom row) outperforms other baselines, across various datasets.

examples per class according to the exponential function $n'_i = n_i \mu^i$, where n_i is the original number of examples for class i, n'_i is the new number of examples per class, and $\mu < 1$ is a scaling factor. Then, we define the imbalance factor $\rho = n'_0 / n'_K$, which is the ratio of the number of examples in the largest class (n'_0) to the smallest class (n'_K). For the **CIFAR-10-LT** and **CIFAR-100-LT** dataset, we construct long-tailed versions of the datasets with imbalance factor $\rho = 100$. **ImageNet-LT** contains 115,846 training examples and 1,000 classes, with imbalance factor $\rho = 256$. **iNaturalist-2018** contains 435,713 images from 8,142 classes, and the imbalance factor is $\rho = 500$. These choices follow that of [50]. For all datasets, we split the long-tailed training set into 80% training and 20% validation during the search phase (Figure 1b).

Implementation. In both CIFAR datasets, the lower-level optimization trains a ResNet-32 model with standard mini-batch stochastic gradient decent (SGD) using learning rate 0.1, momentum 0.9, and weight decay $1e-4$, over 300 epochs. The learning rate decays at epochs 220 and 260 with a factor 0.1. The upper-level hyper-parameter optimization computes the hyper-gradients via implicit differentiation. Because the hyper-gradient is mostly meaningful when the network achieves near zero loss (Thm 1 of [43]), we start the upper optimization after 120 epochs of the lower-level optimization, using SGD with initial learning rate 0.01, momentum 0.9, and weight decay $1e-4$. For CIFAR-LT, 20 hyper-parameters are trained, corresponding to $\boldsymbol{l}$ and $\boldsymbol{\Delta}$ for all classes. For CIFAR-100, because the size of validation data in minority classes can be too small (e.g., only one example in a tail class), as visualized in Figure 3(a), we gather classes of similar frequencies into clusters of size 10 to share the same hyper-parameters (i.e., the values and updates of (l_y, Δ_y)'s). Similarly, for ImageNet-LT, we gather classes into clusters of size 10, and for iNaturalist, we gather classes into clusters of size 40. For ImageNet-LT and iNaturalist, following previous work [50], we use ResNet-50 and SGD for the lower and upper optimizations, and the same learning rate as CIFAR-LT over 150 epochs. We train the network for 40 epochs to warm up before the loss function design starts. The learning rate decays by a factor 0.1 at epochs 80 and 120.

Personalized Data Augmentation (PDA). For PDA, we utilize the AutoAugment [12] policy space and apply a bilevel search for the augmentation policy. Our approach follows existing differentiable augmentation strategies (e.g, [23]); however, we train separate policies for each class cluster to ensure that the resulting policies can adjust to class frequencies. Due to space limitations, please see supplementary materials for further details.

Results and discussion. We compared our methods with the state-of-the-art long-tail learning methods. Table 1 shows the results of our experiments where the design space is parametric CE (4.1). In the first part of the table, we conduct experiments for three baseline methods: normal CE, LDAM [8] and Logit Adjustment loss with temperature parameter $\tau = 1$ [50]. The latter choice guarantees Fisher consistency. In the second part of the Table 1, we study Algo. 1 with design spaces $\boldsymbol{l}$, $\boldsymbol{\Delta}$, and $\boldsymbol{l}\&\boldsymbol{\Delta}$. The first version of Algo. 1 in Table 1 tunes the LA loss parameter τ where $\boldsymbol{l}$ is parameterized by a single scalar τ as $l_y = \tau \log(\pi_y)$. The next three versions of Algo. 1 consider tuning $\boldsymbol{l}$, $\boldsymbol{\Delta}$, $\boldsymbol{l}\&\boldsymbol{\Delta}$ respectively (Figure 3b-d shows the evolution of the $\boldsymbol{l}$ and $\boldsymbol{\Delta}$ parameters during the optimization). Finally, in last version of Algo. 1, the loss design is initialized with LA loss with $\tau = 1$ (rather than balanced CE). The takeaway from these results is that our approach consistently leads to a superior balanced accuracy objective. That said, tuning the LA loss alone is highly competitive with optimizing $\boldsymbol{\Delta}$ and $\boldsymbol{l}$ alone (in fact, strictly better for CIFAR-10-LT, indicating Algo. 1 does not always converge to the optimal design). Importantly, when combining $\boldsymbol{l}\&\boldsymbol{\Delta}$, our algorithm is able to design a better loss function and outperform all rows across all benchmarks. Finally, when the algorithm

Method	CIFAR-10-LT	CIFAR100-LT	ImageNet-LT
MADAO [23]	24.39	59.10	59.92
Algo. 1: $\boldsymbol{\alpha} \leftarrow$PDA	22.53	58.55	58.77
Algo. 1: $\boldsymbol{\alpha} \leftarrow$PDA, $\boldsymbol{\Delta}\&\boldsymbol{l}$	20.76	56.49	52.11

Table 2: The result of personalized data optimization.

Source\Target	CIFAR-10-LT	CIFAR100-LT	ImageNet-LT
CIFAR-10-LT	21.39	58.12	56.13
CIFAR100-LT	22.32	56.77	55.89
ImageNet-LT	23.85	59.17	52.90

Table 3: The results of hyper-parameter transfer.

further is initialized with LA loss, the performance further improves accuracy, demonstrating that warm-starting with good designs improves performance.

In Table 2, we study the benefits of data augmentation, following our intuitions from Lemma 2. We compare to the differentiable augmentation baseline of MADAO [23] which trains a single policy for the full dataset. PDA is a personalized variation of MADAO and leads to noticeable improvement across all benchmarks (most noticeably in CIFAR-10-LT). More importantly, the last line of the table demonstrates that PDA can be synergistically combined with the parametric CE (4.1) which leads to further improvements. Finally, in Table 3, we investigate the transferability of our loss design (including augmentation). Here, a class within the new dataset uses the loss function designed for the closest class from the old dataset, where closest means the most similar class frequency in terms of percentile (when all classes of both datasets are sorted). These results demonstrate that AutoBalance designs transferable loss functions; e.g., loss functions transferred from CIFAR-LT to ImageNet have only slight performance degradation, compared to training the loss from scratch (the diagonals).

6 Approaches and Evaluations for Imbalanced Groups

While Section 5 focuses on the fundamental challenge of balanced error minimization, a more ambitious goal is optimizing generic fairness-seeking objectives. In this section, we study accuracy-fairness tradeoffs by examining the pareto-frontiers of the DEO (3.1), group-balanced error, and standard error. We also investigate group-balanced risk defined as $\mathcal{L}_{\text{bal}}^{\mathcal{G}}(f) = \frac{1}{KG}\sum_{k=1}^{K}\sum_{j=1}^{G}\mathcal{L}_{k,j}(f)$. Note that this definition treats each (class, group) pair as its own (sub)group. Throughout, we explicitly set the loss to cross-entropy for clarity, thus we use CE, $\text{CE}_{\text{bal}}^{\mathcal{G}}$, CE_{DEO} to refer to $\mathcal{L}$, $\mathcal{L}_{\text{bal}}^{\mathcal{G}}$, $\mathcal{L}_{\text{DEO}}$.

Validation (upper-level) loss function. In Algo. 1, we set $\mathcal{L}_{\text{UP}} = (1-\lambda)\cdot\text{CE} + \lambda\cdot\text{CE}_{\text{DEO}}$ for varying $0 \le \lambda \le 1$. The parameter λ enables a trade-off between accuracy and fairness.

Group-sensitive training loss design. The parametric cross-entropy (CE) can be extended to (class, group) imbalance by extending hyper-parameter $\boldsymbol{\alpha}$ to $[K]\times[G]$ variables $\boldsymbol{w}, \boldsymbol{l}, \boldsymbol{\Delta} \in \mathrm{R}^{[K]\times[G]}$ generalizing (4.1), (4.2). This leads us to the following design:

$$\ell_{low}(y, g, f(\boldsymbol{x}); \boldsymbol{\alpha}) = -w_{yg}\log\left(\frac{e^{\sigma(\Delta_{yg})f_y(\boldsymbol{x})+\iota_{yg}}}{\sum_{k\in[K]} e^{\sigma(\Delta_{kg})f_k(\boldsymbol{x})+\iota_{kg}}}\right). \tag{6.1}$$

Here, w_{yg} applies weighted CE, while Δ_{yg} and ι_{yg} are logit adjustments for different (class, groups). Note that a similar group-sensitive loss is proposed in [36] for binary classification.

Baselines. We will compare Algo. 1 with training loss functions parameterized via $(1-\lambda)\cdot\text{CE}+\lambda\cdot\mathcal{L}_{\text{reg}}$. Here $\mathcal{L}_{\text{reg}}$ is a fairness-promoting regularization. Specifically, as displayed in Table 4 and Figure 4, we will set $\mathcal{L}_{\text{reg}}$ to be $\text{CE}_{\text{bal}}^{\mathcal{G}}$, CE_{DEO} and Group LA. "Group LA" is a natural generalization of the LA loss to group-sensitive setting; it chooses weights $w_g = 1/\bar{\boldsymbol{\pi}}_g$ to balance group frequencies and then applies logit-adjustment with $\tau = 1$ over the classes conditioned on the group-membership: $\ell(y, g, f(\boldsymbol{x})) = -\frac{1}{G\bar{\boldsymbol{\pi}}_g}\log\left(\frac{e^{f_y(\boldsymbol{x})+\tau\log\pi_{yg}}}{\sum_{k\in[K]} e^{f_k(\boldsymbol{x})+\tau\log\pi_{kg}}}\right)$.

Datasets. We experiment with the modified Waterbird dataset [54]. The goal is to correctly classify the bird type despite the spurious correlations due to the image background. The distribution of the original data is as follows. The binary classes $k \in \{-,+\}$ correspond to $\{\text{waterbird}, \text{landbird}\}$, and the groups $[G] = \{1, 2\}$ correspond to $\{\text{land background}, \text{water background}\}$. The fraction of data in each (class, group) pair is $\boldsymbol{\pi}_{-,2} = 0.22$, $\boldsymbol{\pi}_{-,1} = 0.012$, $\boldsymbol{\pi}_{+,2} = 0.038$, and $\boldsymbol{\pi}_{+,1} = 0.73$. The landbird on the water background ($\{+,2\}$) and the waterbird on the land background ($\{-,1\}$) are minority sub-groups within their respective classes. The test set, following [54], has equally allocated bird types on different backgrounds, i.e., $\boldsymbol{\pi}_{\pm,j} = 0.25$. As the test dataset is balanced, the standard classification error $\mathcal{E}(f)$ is defined to be the weighted error $\mathcal{E}(f) = \boldsymbol{\pi}_{y,g}\mathcal{E}_{\text{y,g}}(f)$.

Implementation. We follow the feature extraction method from [54], where x_i are 512-dimensional ResNet18 features. When using Algo. 1, we split the original training data into 50% training and

Loss function	Balanced Error	Worst (class, group) error	DEO
Cross entropy (CE)	23.38	43.25	33.75
CE_{bal}	20.83	36.67	20.25
Group-LA loss	22.83	40.50	29.33
CE_{DEO}	19.29	35.17	25.25
$0.1 \cdot \text{CE} + 0.9 \cdot \text{CE}_{\text{DEO}}$ ($\lambda = 0.1$)	20.06	31.67	26.25
Algo. 1: with $\lambda = 0.1$	**15.13**	**30.33**	**4.25**

Table 4: Comparison of fairness metrics for group-imbalanced experiments. The first five rows are different training loss choices, where CE_{bal}, Group-LA, and CE_{DEO} promote group fairness. The last row is Algo. 1, which designs training loss for the validation loss choice of $0.1 \cdot \text{CE} + 0.9 \cdot \text{CE}_{\text{DEO}}$. We note that, DEO can be trivially minimized by always predicting the same class. To avoid this, we use a mild amount of CE loss with $\lambda = 0.1$ in Algo. 1.

50% validation. The search phase uses 150 epochs of warm up followed by 350 epochs of bilevel optimization. The remaining implementation details are similar to Section 5.

Results and discussion. We consider various fairness-related metrics, including the worst (class, group) error, DEO $\mathcal{E}_{\text{DEO}}(f)$ and the balanced error $\mathcal{E}^{\mathcal{G}}_{\text{bal}}(f)$.We seek to understand whether AutoBalance algorithm can improve performance on the test set compared to the baseline training loss functions of the form $(1-\lambda) \cdot \text{CE} + \lambda \cdot \mathcal{L}_{\text{reg}}$. In Figure 4, we show the influence of the parameter λ where $\mathcal{L}_{\text{reg}}$ is chosen to be CE_{DEO}, CE_{bal}, or Group-LA (each point on the plot represents a different λ value). As we sweep across values of λ, there arises a tradeoff between standard classification error $\mathcal{E}(f)$ and the fairness metrics. We observe that Algo. 1 significantly Pareto-dominates alternative approaches, for example achieving lower DEO or balanced error for the same standard error. This demonstrates the value of automatic loss function design for a rich class of fairness-seeking objectives.

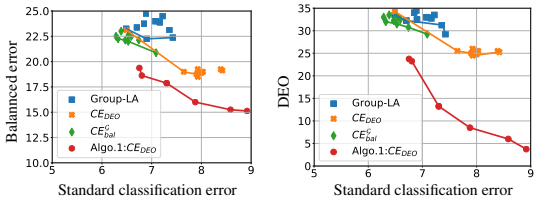


Figure 4: Waterbirds fairness-accuracy tradeoffs for parametrized loss designs $(1-\lambda) \cdot \text{CE} + \lambda \cdot \mathcal{L}_{\text{reg}}$, for different $\mathcal{L}_{\text{reg}}$ choices. Group-balanced error $\mathcal{E}^{\mathcal{G}}(f)$ (left) and DEO $\mathcal{E}_{\text{DEO}}(f)$ (right) are plotted as a function of the misclassification error $\mathcal{E}(f)$. Algo. 1 exhibits a noticeably better tradeoff curve as it uses a DEO-based validation objective to design an optimized training loss function.

Next, in Table 4, we solely focus on optimizing the fairness objectives (rather than standard error). Thus, we simply set $\lambda = 0$ and compare against CE_{DEO}, CE_{bal}, Group-LA as the baseline approaches (without blending CE). We also display the outcome of Algo. 1 with $\lambda = 0.1$. Similar too Figure 4, our approach outperforms all baselines for all metrics. The performance gap is particularly noticeable when it comes to DEO (4.25% for Algo. 1, vs 20.25% for the best baseline).

7 Conclusions and Future Directions

This work provides an optimization-based approach to automatically design loss functions to address imbalanced learning problems. Our algorithm consistently outperforms, or is at least competitive with, the state-of-the-art approaches for optimizing balanced accuracy. Importantly, our approach is not restricted to imbalanced classes or specific objectives, and can achieve good tradeoffs between (accuracy, fairness) on the Pareto frontier. We also provide theoretical insights on certain algorithmic aspects including loss function design, data augmentation, and train-validation split.

Potential Limitations, Negative Societal Impacts, & Precautions: Our algorithmic approach can be considered within the realm of automated machine learning literature (AutoML) [25]. AutoML algorithms often optimize the model performance, thus reducing the need for engineering expertise at the expense of increased computational cost and increased carbon footprint. For instance, our procedure is computationally more intensive compared to the theory-inspired loss function prescriptions of [50, 8]. A related limitation is that Algo. 1 can be brittle in extremely imbalanced scenarios with very few samples per class. We took the several steps to help mitigate such issues: first, our algorithm is initialized with a Bayes consistent loss function to provide a warm-start (such as the proposal of [50]). Second, we reduce the hyper-parameter search space by grouping classes with similar frequencies (to help with brittleness). Finally, evaluations show that the designed loss functions are transferable, and hence our algorithm does does not have to train from scratch for a new dataset.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] We use computing server with 2 RTX2080 Ti GPU.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]