Calibrating Predictions to Decisions: A Novel Approach to Multi-Class Calibration

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Abstract

When facing uncertainty, decision-makers want predictions they can trust. A machine learning provider can convey confidence to decision-makers by guaranteeing their predictions are distribution calibrated— amongst the inputs that receive a predicted vector of class probabilities q, the actual distribution over classes is given by q. For multi-class prediction problems, however, directly optimizing predictions under distribution calibration tends to be infeasible, requiring sample complexity that grows exponentially in the number of classes C. In this work, we introduce a new notion—*decision calibration*—that requires the predicted distribution and true distribution over classes to be "indistinguishable" to downstream decision-makers. This perspective gives a new characterization of distribution calibration: a predictor is distribution calibrated if and only if it is decision calibrated with respect to *all* decision-makers. Our main result shows that under a mild restriction, unlike distribution calibration, decision calibration is actually feasible. We design a recalibration algorithm that provably achieves decision calibration efficiently, provided that the decision-makers have a bounded number of actions (e.g., polynomial in C). We validate our recalibration algorithm empirically: compared to existing methods, decision calibration improves decision-making on skin lesion and ImageNet classification with modern neural network predictors.

1 Introduction

Machine learning predictions are increasingly employed by downstream decision makers who have little or no visibility on how the models were designed and trained. In high-stakes settings, such as healthcare applications, decision makers want predictions they can trust. For example, suppose a machine learning service offers a supervised learning model to healthcare providers that claims to predict the probability of various skin diseases, given an image of a lesion. Each healthcare provider may want assurance that the model's predictions lead to beneficial decisions, according to their own loss function. Concretely, the healthcare providers may reasonably worry that the model was trained using a loss function different than their own. This mismatch is often inevitable because the ML service may provide the same prediction model to many healthcare providers, which may have different treatment options available and loss functions. Even the same healthcare provider could have different loss functions throughout time, due to changes in treatment availability.

If predicted probabilities were perfect—exactly matching the corresponding empirical frequencies—the issue would not arise because they would lead to optimal decision making regardless of the loss function or task considered by downstream decision makers. In practice, however, predicted

probabilities are never perfect. To address this, the healthcare providers may insist that the prediction function be at least *distribution calibrated*, requiring that amongst the inputs that receive predicted class probabilities q, the actual distribution over classes is q. This solves the trust issue because among the patients who receive prediction q, the healthcare providers knows their true label distribution (which is also q) and hence know the true expected loss of a treatment on these patients. Unfortunately, to achieve distribution calibration, we need to reason about the set of individuals x who receive prediction q, for *every* possible predicted q. As the number of distinct predictions may naturally grow exponentially in the number of classes C, the amount of data needed to accurately certify distribution calibration tends to be prohibitive. Due to this statistical barrier, most work on obtaining calibrated multi-class predictions focuses on obtaining relaxed variants of calibration. These include *confidence calibration* (Guo et al., 2017), which calibrates predictions only over the most likely class, and *classwise calibration* (Kull et al., 2019), which calibrates predictions for each class marginally. While feasible, intuitively, these notions are significantly weaker than distribution calibration and do not address the trust issue highlighted above. Is there a calibration notion that addresses the issue of trust, but can also be verified and achieved efficiently? Our paper answers this question affirmatively.

Our Contributions. We introduce a new notion of calibration—*decision calibration*—where we take the perspective of potential decision-makers: the only differences in predictions that matter are those that could lead to different decisions. Inspired by Dwork et al. (2021), we formalize this intuition by requiring that predictions are "indistinguishable" from the true outcomes, according to a collection of decision-makers.

First, we show that all prior notions of calibration can be characterized as variants of decision calibration under different decision-makers. This framing explains the strengths and weakness of existing notions of calibration. For example, we show that a predictor is distribution calibrated if and only if it is decision calibrated with respect to *all* loss functions and decision rules. This characterization demonstrates why distribution calibration is so challenging: achieving distribution calibration requires simultaneously reasoning about all possible decision tasks.

Distribution calibration can guarantee decision calibration with respect to decision rules that choose between exponentially (in number of classes C) many actions. In practice, however, decision-makers typically choose from a bounded (or slowly-growing as a function of C) set of actions. Our main contribution is an algorithm that **guarantees decision calibration for such realistic decision-makers**. In particular, we give a sample-efficient algorithm that takes a pre-trained predictor and post-processes it to achieve decision calibration with respect to *all* decision-makers choosing from a bounded set of actions. Our recalibration procedure does not harm other performance metrics, and slightly improves accuracy and likelihood of the predictions. Empirically, we use our algorithm to recalibrate deep network predictors on two large scale datasets: skin lesion classification (HAM10000) and Imagenet. Our recalibration algorithm improves decision making, and allow for significantly more accurate loss estimation compared to existing recalibration methods.

2 Background

2.1 Setup and Notation

We consider the prediction problem with random variables X and Y. $X \in \mathcal{X}$ denotes the input features, and $Y \in \mathcal{Y}$ denotes the label. We focus on classification where $\mathcal{Y} = \{(1, 0, \cdots, 0), (0, 1, \cdots, 0), \cdots, (0, 0, \cdots, 1)\}$ where each $y \in \mathcal{Y}$ is a one-hot vector with $C \in \mathbb{N}$ classes. A probability prediction function is a map $\hat{p} : \mathcal{X} \to \Delta^C$ where Δ^C is the C-dimensional simplex. We use $p^* : \mathcal{X} \to \Delta^C$ to denote the true conditional probability, i.e. $p^*(x) = \mathbb{E}[Y \mid X = x]$.

2.2 Decision Making Tasks and Loss Functions

We formalize a decision making task as a utility maximization / loss minimization problem. The decision maker has some set of available actions $\mathcal{A}$ and a loss function $\ell : \mathcal{Y} \times \mathcal{A} \to \mathbb{R}$. In this paper we assume the loss function does not directly depend on the input features X. For notational simplicity we often refer to a (action set, loss function) pair $(\mathcal{A}, \ell)$ only by the loss function ℓ: the set of actions $\mathcal{A}$ is implicitly defined by the domain of ℓ. We denote the set of all possible loss functions as $\mathcal{L}_{\text{all}} = \{\ell : \mathcal{Y} \times \mathcal{A} \to \mathbb{R}\}$.

We treat all action sets $\mathcal{A}$ with the same cardinality as the same set — they are equivalent up to renaming the actions. A convenient way to think about this is that we only consider actions sets $\mathcal{A} \in \{[1], [2], \cdots, [K], \cdots, \mathbb{N}, \mathbb{R}\}$ where $[K] = \{1, \cdots, K\}$.

2.3 Bayes Decision

Given some predicted probability $\hat{p}(X)$ on Y, a decision maker selects an action in $\mathcal{A}$. We assume that the decision maker selects the action based on the predicted probability, that is we define a decision function as any map from the predicted probability to an action $\delta : \Delta^C \to \mathcal{A}$. and denote by $\mathbb{\Delta}_{\text{all}}$ as the set of all decision functions.

Typically a decision maker selects the action that minimizes the expected loss (under the predicted probability). This is formalized by the following definition

Definition 1 (Bayes Decision)**.** *Choose any $\ell \in \mathcal{L}_{\text{all}}$ with corresponding action space $\mathcal{A}$ and prediction $\hat{p}$, define the Bayes decision function as $\delta_\ell(\hat{p}(x)) = \arg\inf_{a \in \mathcal{A}} \mathbb{E}_{\hat{Y} \sim \hat{p}(x)}[\ell(\hat{Y}, a)]$. For any subset $\mathcal{L} \subset \mathcal{L}_{\text{all}}$ denote the set of all Bayes decision functions as $\mathbb{\Delta}_{\mathcal{L}} := \{\delta_\ell, \ell \in \mathcal{L}\}$.*

3 Calibration: A Decision Making Perspective

In our setup, the decision maker outsources the prediction task and uses a prediction function $\hat{p}$ provided by a third-party forecaster (e.g., an ML Prediction API). A decision maker would ideally want to train a prediction function $\hat{p}$ (or even more directly, a decision rule) to minimize the decision loss, however, this is often overly expensive, and decision makers often prefer to settle for off-the-shelf prediction functions due to resource constraints. A generic prediction function will have to be trained by a forecaster without knowledge of the exact loss ℓ downstream decision makers will use (or worse, will be used by multiple decision-makers with different loss functions). For example, prediction functions are often trained to minimize standard objectives such as L2 error or log likelihood.

This would not be an issue if the forecaster can perfectly learn the true distribution (i.e. $\hat{p}(X) = p^*(X)$ almost surely). Unfortunately, predictions are usually imperfect, and a prediction function trained to minimize L2 or log likelihood loss might or might not perform well on downstream tasks depending on the loss ℓ used. To mitigate concerns about the performance of the prediction function, the forecasters might offer (or decision makers might demand) performance guarantees applicable to decision makers with any loss function $\ell \in \mathcal{L}_{\text{all}}$. We also consider the case where the forecaster provides guarantees for decision makers whose loss functions come from some subset $\mathcal{L} \subset \mathcal{L}_{\text{all}}$.

3.1 Decision Calibration

First and foremost, a decision maker wants assurance that making decisions based on the prediction function $\hat{p}$ give low expected loss. Specifically, a decision maker with loss function ℓ naturally wants to use the Bayes decision rule δ_ℓ, so she wants δ_ℓ to incur a lower loss compared to alternative decision rules. Second, the decision maker wants to know how much loss is going to be incurred (before the actions are deployed and outcomes are revealed); the decision maker does not want to incur any additional loss in surprise that she has not prepared for.

To capture these desiderata we formalize a definition based on the following intuition: suppose a decision maker with some loss function ℓ considers a decision rule $\delta \in \mathbb{\Delta}_{\text{all}}$ (that may or may not be the Bayes decision rule), the decision maker should be able to correctly compute the expected loss of using δ to make decisions.

Definition 2 (Decision Calibration)**.** *For any set of loss functions $\mathcal{L} \subset \mathcal{L}_{\text{all}}$ and set of decision rules $\mathbb{\Delta} \subset \mathbb{\Delta}_{\text{all}} := \{\Delta^C \to \mathcal{A}\}$, we say that a prediction $\hat{p}$ is $(\mathcal{L}; \mathbb{\Delta})$-decision calibrated (with respect to p^*) if $\forall \ell \in \mathcal{L}$ and $\delta \in \mathbb{\Delta}$ with the same action space $\mathcal{A}$* [1]

$$\mathbb{E}_X \mathbb{E}_{\hat{Y} \sim \hat{p}(X)}[\ell(\hat{Y}, \delta(\hat{p}(X)))] = \mathbb{E}_X \mathbb{E}_{Y \sim p^*(X)}[\ell(Y, \delta(\hat{p}(X)))] \tag{1}$$

In particular, we say $\hat{p}$ is $\mathcal{L}$-decision calibrated if it is $(\mathcal{L}; \mathbb{\Delta}_{\mathcal{L}})$-decision calibrated.

[1] We require ℓ and δ to have the same action space $\mathcal{A}$ for type check reasons. Eq.(1) only has meaning if the loss ℓ and decision rule $\mathbb{\Delta}$ are associated with the same action space $\mathcal{A}$.

Existing Calibration Definitions	Associated Loss Functions
Confidence Calibration (Guo et al., 2017) $\Pr[Y = \arg\max \hat{p}(X) \mid \max \hat{p}(X) = \beta] = \beta$ $\forall \beta \in [0, 1]$	$\mathcal{L}_r := \left\{ \begin{array}{l} \ell(y, a) = \mathbb{I}(y \neq a \cap a \neq \perp) + \beta \mathbb{I}(a = \perp) : \\ a \in \mathcal{Y} \cup \{\perp\}, \forall \beta \in [0, 1] \end{array} \right\}$
Classwise Calibration (Kull et al., 2019) $\mathbb{E}[Y_c \mid \hat{p}_c(X) = \beta] = \beta, \forall c \in [C], \forall \beta \in [0, 1]$	$\mathcal{L}_{cr} := \left\{ \begin{array}{l} \ell(y, a) = \mathbb{I}(a = \perp) + \beta_1 \mathbb{I}(y = c, a = T) \\ \qquad\qquad + \beta_2 \mathbb{I}(y \neq c, a = F) : \\ a \in \{T, F, \perp\}, \forall \beta_1, \beta_2 \in \mathbb{R}, c \in [C] \end{array} \right\}$
Distribution Calibration (Kull & Flach, 2015) $\mathbb{E}[Y \mid \hat{p}(X) = q] = q, \forall q \in \Delta^C$	$\mathcal{L}_{\text{all}} = \{\ell : \mathcal{Y} \times \mathcal{A} \mapsto \mathbb{R}\}$

Table 1: A prediction function $\hat{p}$ satisfies the calibration definitions on the left if and only if it satisfies $\mathcal{L}$-decision calibration for the loss function families on the right (Theorem 1).

The left hand side of Eq.(1) is the "simulated" loss where the outcome $\hat{Y}$ is hypothetically drawn from the predicted distribution. The decision maker can compute this just by knowing the input features X and without knowing the outcome Y. The right hand side of Eq.(1) is the true loss that the decision maker incurs in reality if she uses the decision rule δ. Note that Eq.(1) should not be mis-interpreted as guarantees about individual decisions; Eq.(1) only looks at the average loss when X, Y is a random draw from the population. Individual guarantees are usually impossible (Zhao & Ermon, 2021).

We define the special notion of $\mathcal{L}$-decision calibrated because given a set of loss functions $\mathcal{L}$, we are often only interested in the associated Bayes decision rules $\mathbb{\Delta}_{\mathcal{L}}$, i.e. the set of decision rules that are optimal under *some* loss function. For the rest of the paper we focus on $\mathcal{L}$-decision calibration for simplicity. $\mathcal{L}$-decision calibration can capture the desiderata we discussed above

Proposition 1. *If a prediction function $\hat{p}$ is $\mathcal{L}$-decision calibrated, then it satisfies*

$$\forall \delta' \in \mathbb{\Delta}_{\mathcal{L}}, \mathbb{E}_X \mathbb{E}_{Y \sim p^*(X)}[\ell(Y, \delta_\ell(\hat{p}(X)))] \leq \mathbb{E}_X \mathbb{E}_{Y \sim p^*(X)}[\ell(Y, \delta'(\hat{p}(X)))] \quad \textit{(No regret)}$$

$$\mathbb{E}_X \mathbb{E}_{\hat{Y} \sim \hat{p}(X)}[\ell(\hat{Y}, \delta_\ell(\hat{p}(X)))] = \mathbb{E}_X \mathbb{E}_{Y \sim p^*(X)}[\ell(Y, \delta_\ell(\hat{p}(X)))] \quad \textit{(Accurate loss estimation)}$$

No regret states that the Bayes decision rule δ_ℓ is not worse than any alternative decision rule $\delta' \in \mathbb{\Delta}_{\mathcal{L}}$. Note we do not guarantee no regret with respect to any decision rule in $\mathbb{\Delta}_{\text{all}}$. This is going to be a mild restriction because we will achieve decision calibration with respect to a very large class of loss functions $\mathcal{L}$ (any loss function with a bounded number of actions) such that $\mathbb{\Delta}_{\mathcal{L}}$ will consist of almost all realistic decision rules.

Accurate loss estimation states that for the Bayes decision rule δ_ℓ, the simulated loss on the left hand side (which the decision maker can compute before the outcomes are revealed) equals the true loss on the right hand side. This ensures that the decision maker knows the expected loss it's going to incur and can prepare for it.

In practice, the forecaster chooses some set $\mathcal{L}$ to achieve $\mathcal{L}$-decision calibration, and advertise it to decision makers. A decision makers can then check whether their loss function ℓ belongs to the advertised set $\mathcal{L}$. If it does, the decision maker should be confident that the Bayes decision rule δ_ℓ has low loss compared to alternatives in $\mathbb{\Delta}_{\mathcal{L}}$, and they can know in advance the loss that will be incurred.

3.2 Decision Calibration Generalizes Existing Notions of Calibration

This section connects decision calibration with existing notions of calibration in Table 1. Decision calibration provides a unified view of existing notions of calibration as the following theorem shows.

Theorem 1 (Calibration Equivalence)**.** *For any true distribution p^*, and for the loss function sets $\mathcal{L}_r, \mathcal{L}_{cr}$ defined in Table 1, a prediction function $\hat{p}$ is*

- *confidence calibrated iff it is $\mathcal{L}_r$-decision calibrated.*
- *classwise calibrated iff it is $\mathcal{L}_{cr}$-decision calibrated.*
- *distribution calibrated iff it is $\mathcal{L}_{all}$-decision calibrated.*

For proof of this theorem see Appendix D. In Theorem 1 and Table 1, confidence and classwise calibration are weak notions of calibration; correspondingly the loss function families $\mathcal{L}_r$ and $\mathcal{L}_{\text{cr}}$ are also very restricted. For example, confidence calibration only requires that the top-1 accuracy

$\Pr[Y = \arg\max \hat{p}(X)]$ matches the predicted top-1 probability $\max \hat{p}(X)$. Correspondingly, $\mathcal{L}_r$ consists of loss functions for the refrained prediction task: a decision maker chooses between reporting a class label, or reporting "I don't know," denoted $\perp$. If the decision maker reports a class label, she incurs a loss of 1 if the reported class label is incorrect; if the decision maker reports "I don't know" then she incurs a loss of $\beta < 1$. Even though such decision tasks are useful, they only account for a tiny subset of all possible tasks that are interesting to decision makers.

On the other hand, distribution calibration (i.e. $\mathbb{E}[Y \mid \hat{p}(X) = q] = q, \forall q \in \Delta^C$) is equivalent to $\mathcal{L}_{\text{all}}$-decision calibration. This means that decision makers with any loss functions are guaranteed the properties of no regret and accurate loss estimation as in Proposition 1. Unfortunately, distribution calibration is very challenging to verify or achieve. To understand the challenges, consider certifying whether a given predictor $\hat{p}$ is distribution calibrated. Because we need to reason about the conditional distribution $\mathbb{E}[Y \mid \hat{p}(X) = q]$ for every q that $\hat{p}$ can predict (i.e. the support of $\hat{p}$), the necessary sample complexity grows linearly in the support of $\hat{p}$. Of course, for a trivial predictors that map all inputs x to the same prediction q_0 (i.e. $\hat{p}(x) = q_0, \forall x \in \mathcal{X}$) distribution calibration is easy to certify (Widmann et al., 2019), but such predictors have no practical use, and informative predictors naturally have exponentially large (in the number of classes C) support.

Our characterization of distribution calibration further sheds light on why it is so difficult to achieve. $\mathcal{L}_{\text{all}}$ consists of *all* loss function, including all loss functions $\ell : \mathcal{Y} \times \mathcal{A} \to \mathbb{R}$ whose action space $\mathcal{A}$ contains exponentially many elements (e.g. $|\mathcal{A}| = 2^C$). The corresponding decision rules $\delta \in \mathbb{\Delta}_{\mathcal{L}_{\text{all}}} : \Delta^C \to \mathcal{A}$ may also map Δ^C to exponentially many possible values. Intuitively, a predictor that guarantees $\mathcal{L}_{\text{all}}$-decision calibration guarantees accurate loss estimation even when the losses and decisions are specified separately for each $q \in \Delta^C$ (just as distribution calibration conditions on $\hat{p}(X) = q$ for each $q \in \Delta^C$). Enforcing Definition 2 for such complex loss functions and decision rules is naturally difficult. But we argue that it may also be *unnecessary* in many contexts, as realistic decision makers often choose from a bounded set of discrete actions.

4 Achieving Decision Calibration with PAC Guarantees

In this section, we consider obtaining decision calibration for all loss functions defined over a bounded number of actions $K \in \mathbb{N}$. Formally, let $\mathcal{L}^K$ be the set of all loss functions with K possible actions, i.e. $\mathcal{L}^K = \{\ell : \mathcal{Y} \times \mathcal{A} \to \mathbb{R}, |\mathcal{A}| = K\} \subset \mathcal{L}_{\text{all}}$. In practice, decision-makers are unlikely to have an unbounded number of actions, so for most realistic settings, the relevant losses will be in $\mathcal{L}^K$ for some reasonable $K \in \mathbb{N}$. In the remainder of this section, we demonstrate an efficient strategy for obtaining approximately $\mathcal{L}^K$-decision calibrated predictors. In Appendix B we also explore the theoretical connection between $\mathcal{L}^K$-decision calibration and distribution calibration to show that $\mathcal{L}^K$-decision calibration improves upon distribution calibration in almost every way.

4.1 Approximate $\mathcal{L}^K$ Decision Calibration is Verifiable and Achievable

Decision calibration in Definition 2 usually cannot be achieved perfectly. The definition has to be relaxed to allow for statistical and numerical errors. To meaningfully define approximate calibration we must assume that the loss functions are bounded, i.e. no outcome $y \in \mathcal{Y}$ and action $a \in \mathcal{A}$ can incur an infinite loss. In particular, we bound ℓ by its 2-norm $\max_a \|\ell(\cdot, a)\|_2 := \max_a \sqrt{\sum_{y \in \mathcal{Y}} \ell(y, a)^2}$. [2]

Now we can proceed to define approximate decision calibration. In particular, we compare the difference between the two sides in Eq.(1) of Definition 2 with the maximum size of the loss function.

Definition 3 (Approximate decision calibration)**.** *A prediction function $\hat{p}$ is $(\mathcal{L}, \epsilon)$-decision calibrated (with respect to p^*) if $\forall \ell \in \mathcal{L}$ and $\delta \in \mathbb{\Delta}_{\mathcal{L}}$*

$$\left| \mathbb{E}[\ell(\hat{Y}, \delta(\hat{p}(X)))] - \mathbb{E}[\ell(Y, \delta(\hat{p}(X)))] \right| \leq \epsilon \sup_{a \in \mathcal{A}} \|\ell(\cdot, a)\|_2 \tag{2}$$

Definition 3 is a relaxation of Definition 2: if a prediction function is $(\mathcal{L}, 0)$-decision calibrated, then it is $\mathcal{L}$-decision calibrated (Definition 2).

[2] The choice of 2-norm is for convenience. All p-norms are equivalent up to a multiplicative factor polynomial in C, so our main theorem (Theorem 2) still hold for any p-norms up to the polynomial factor.

The main observation in our paper is that for the set of loss functions with K actions, $(\mathcal{L}^K, \epsilon)$-decision calibration can be verified and achieved with polynomially many samples.

Theorem 2 (Main Theorem, informal)**.** *There is an algorithm, such that for any predictor $\hat{p}$ and given polynomially (in $K, C, 1/\epsilon$) many samples, can with high probability*

1. *correctly decide if $\hat{p}$ satisfies $(\mathcal{L}^K, \epsilon)$-decision calibration*
2. *output a new predictor $\hat{p}'$ that satisfies $(\mathcal{L}^K, \epsilon)$-decision calibration without degrading the original predictions (in terms of L_2 error).*

As with distribution calibration, trivial predictors $\hat{p}(x) \equiv \mathbb{E}[Y], \forall x$ satisfy $(\mathcal{L}^K, 0)$-decision calibration. To maintain a meaningful prediction function we also require "sharpness" which we measure by L_2 error. We guarantee that the L_2 error of $\hat{p}'$ can only *improve* under post-processing; that is, $\mathbb{E}[\|\hat{p}'(X) - Y\|_2^2] \leq \mathbb{E}[\|\hat{p}(X) - Y\|_2^2]$. In fact, the algorithm works by iteratively updating the predictions to make progress in L_2. For rest of this section, we propose concrete algorithms that satisfy Theorem 2.

4.2 Verification of Decision Calibration

This section focuses on the first part of Theorem 2 where we certify $(\mathcal{L}^K, \epsilon)$-decision calibration. A naive approach would use samples to directly estimate

$$\sup_{\delta \in \mathbb{\Delta}_{\mathcal{L}^K}} \sup_{\ell \in \mathcal{L}^K} \left| \mathbb{E}[\ell(\hat{Y}, \delta(\hat{p}(X)))] - \mathbb{E}[\ell(Y, \delta(\hat{p}(X)))] \right| / \left(\sup_{a \in \mathcal{A}} \|\ell(\cdot, a)\|_2 \right) \tag{3}$$

and compare it with ϵ. However, the complexity of this optimization problem poses challenges to analysis. We will make several observations to transform this complex optimization problem to a simple problem that resembles linear classification.

Observation 1. The first observation is that we do not have to take the supremum over $\mathcal{L}^K$ because for any choice of $\delta \in \mathbb{\Delta}$ by simple calculations (details in the Appendix) we have

$$\sup_{\ell \in \mathcal{L}^K} \frac{\left| \mathbb{E}[\ell(\hat{Y}, \delta(\hat{p}(X)))] - \mathbb{E}[\ell(Y, \delta(\hat{p}(X)))] \right|}{\sup_{a \in \mathcal{A}} \|\ell(\cdot, a)\|_2} = \sum_{a=1}^{K} \left\| \mathbb{E}[(\hat{Y} - Y)\mathbb{I}(\delta(\hat{p}(X)) = a)] \right\|_2 \tag{4}$$

Intuitively on the right hand side, δ partitions the probabilities Δ^C based on the optimal decision $\Delta_1 := \{q \in \Delta^C, \mathbb{I}(\delta(q) = 1)\}, \cdots, \Delta_K := \{q \in \Delta^C, \mathbb{I}(\delta(q) = K)\}$. For each partition Δ_k we measure the difference between predicted label and true label *on average*, i.e. we compute $\mathbb{E}[(\hat{Y} - Y)\mathbb{I}(\hat{p}(X) \in \Delta_k)]$.

Observation 2. We observe that the partitions of Δ^C are defined by linear classification boundaries. Formally, we introduce a new notation for the linear multi-class classification functions

$$B^K = \left\{ b_w \mid \forall w \in \mathbb{R}^{K \times C} \right\} \qquad \text{where } b_w(q, a) = \mathbb{I}(a = \arg \sup_{a' \in [K]} \langle q, w_{a'} \rangle) \tag{5}$$

Note that this new classification task is a tool to aid in understanding decision calibration, and bears no relationship with the original prediction task (predicting Y from X). Intuitively w is the weights of a linear classifier; given input features $q \in \Delta^C$ and a candidate class a, b_w outputs an indicator: $b_w(q, a) = 1$ if the optimal decision of q is equal to a and 0 otherwise.

The following equality draws the connection between Eq.(4) and linear classification. The proof is simply a translation from the original notations to the new notations.

$$\sup_{\delta \in \mathbb{\Delta}_{\mathcal{L}^K}} \sum_{a=1}^{K} \left\| \mathbb{E}[(\hat{Y} - Y)\mathbb{I}(\delta(\hat{p}(X))) = a)] \right\|_2 = \sup_{b \in B^K} \sum_{a=1}^{K} \left\| \mathbb{E}[(\hat{Y} - Y) b(\hat{p}(X), a)] \right\|_2 \tag{6}$$

The final outcome of our derivations is the following proposition (Proof in Appendix D.2)

Proposition 2. *$\hat{p}$ satisfies $(\mathcal{L}^K, \epsilon)$-decision calibration if and only if*

$$\sup_{b \in B^K} \sum_{a=1}^{K} \left\| \mathbb{E}[(\hat{Y} - Y) b(\hat{p}(X), a)] \right\|_2 \leq \epsilon \tag{7}$$

In words, $\hat{p}$ satisfies decision calibration if and only if there is no linear classification function that can partition Δ^C into K parts, such that the average difference $\hat{Y} - Y$ (or equivalently $\hat{p}(X) - p^*(X)$) in each partition is large. Theorem 2.1 follows naturally because B^K has low Radamacher complexity, so the left hand side of Eq.(7) can be accurately estimated with polynomially many samples. For a formal statement and proof see Appendix D.2.

The remaining problem is computation. With unlimited compute, we can upper bound Eq.(7) by brute force search over B^K; in practice, we use a surrogate objective optimizable with gradient descent. This is the topic of Section 4.4.

4.3 Recalibration Algorithm

This section discusses the second part of Theorem 2 where we design a post-processing recalibration algorithm. The algorithm is based on the following intuition, inspired by (Hébert-Johnson et al., 2018): given a predictor $\hat{p}$ we find the worst $b \in B^K$ that violates Eq.(7) (line 3 of Algorithm 1); then, we make an update to $\hat{p}$ to minimize the violation of Eq.(7) for the worst b (line 4,5 of Algorithm 1). This process is be repeated until we get a (B^K, ϵ)-decision calibrated prediction (line 2). The sketch of the algorithm is shown in Algorithm 1 and the detailed algorithm is in the Appendix.

Algorithm 1: Recalibration algorithm to achieve $\mathcal{L}^K$ decision calibration.

1 Input current prediction function $\hat{p}$, tolerance ϵ. Initialize $\hat{p}^{(0)} = \hat{p}$;
2 **for** $t = 1, 2, \cdots, T$ *until output* $\hat{p}^{(T)}$ *when it satisfies Eq.(7)* **do**
3 Find $b \in B^K$ that maximizes $\sum_{a=1}^{K} \left\| \mathbb{E}[(Y - \hat{p}^{(t-1)}(X)) b(\hat{p}^{(t-1)}(X), a) \right\|^2$;
4 For each a compute the adjustment $d_a = \mathbb{E}[(Y - \hat{p}^{(t-1)}(X)) b(\hat{p}^{(t-1)}(X), a)]$;
5 Set $\hat{p}^{(t)} : x \mapsto \pi\left(\hat{p}^{(t-1)}(x) + \sum_{a=1}^{K} b(\hat{p}^{(t-1)}(x), a) \cdot d_a\right)$, π is normalizing projection ;
6 **end**

Given a dataset with N samples, the expectations in Algorithm 1 are replaced with empirical averages. The following theorem demonstrates that Algorithm 1 satisfies the conditions stated in Theorem 2.

Theorem 2.2. *Given any input $\hat{p}$ and tolerance ϵ, Algorithm 1 terminates in $O(1/\epsilon^2)$ iterations. Given $O(poly(K, C, \log(1/\delta)))$ samples, with $1 - \delta$ probability Algorithm 1 outputs a $(\mathcal{L}^K, \epsilon)$-decision calibrated prediction function $\hat{p}'$ that satisfies $\mathbb{E}[\|\hat{p}'(X) - Y\|_2^2] \leq \mathbb{E}[\|\hat{p}(X) - Y\|_2^2]$.*

4.4 Relaxation of Decision Calibration for Computational Efficiency

We complete the discussion by addressing the open computational question. Directly optimizing over B^K is difficult, so we instead define the softmax relaxation.

$$\bar{B}^K = \left\{ \bar{b}_w \mid \forall w \in \mathbb{R}^{K \times C} \right\} \qquad \text{where } \bar{b}_w(q, a) = \frac{e^{\langle q, w_a \rangle}}{\sum_{a'} e^{\langle q, w_{a'} \rangle}}$$

The key motivation behind this relaxation is that $\bar{b}_w \in \bar{B}^K$ is now is differentiable in w, so we can optimize over $\bar{B}^K$ using gradient descent. Correspondingly some technical details in Algorithm 1 change to accommodate soft partitions; we address these modifications in Appendix A. Importantly, even when we optimize over $\bar{B}^K$, we still obtain our approximate decision calibration goal.

Proposition 3. *A prediction function $\hat{p}$ is $(\mathcal{L}^K, \epsilon)$-decision calibrated if it satisfies*

$$\sup_{\bar{b} \in \bar{B}^K} \sum_{a=1}^{K} \left\| \mathbb{E}[(\hat{Y} - Y) \bar{b}(\hat{p}(X), a)] \right\|_2 \leq \epsilon \tag{8}$$

5 Empirical Evaluation

5.1 Skin Legion Classification

This experiment materializes our motivating example in the introduction. We aim to show on a real medical prediction dataset, our recalibration algorithm improves both the decision loss and reduces

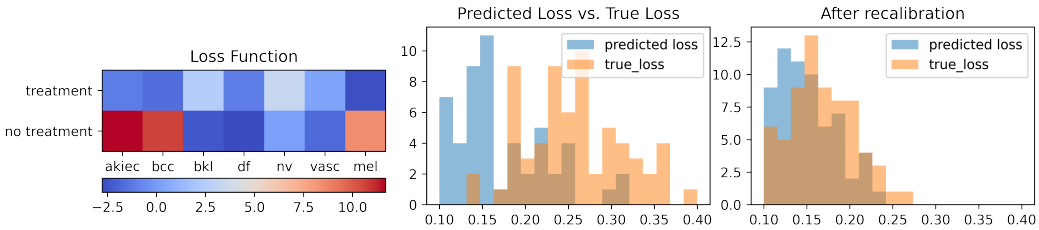

Figure 1: An illustrative example of accurate loss estimation on the HAM10000 dataset. The predictor predicts the probability of 7 skin illness categories (akiec, bcc, ..., mel); the hospital decides between two actions (treatment vs. no treatment). **Left** An example loss function (details not important). Blue indicates low loss and red indicates high loss. For the malignant conditions such as 'akiec' and 'mel', no treatment has high loss (red); for the benign conditions such as 'nv', (unnecessary) treatment has moderate loss. **Middle** Histogram of predicted loss vs. the true loss. The predicted loss is the loss the hospital expected to incur assuming the predicted probabilities are correct under the Bayes decision rule.The true loss is the loss the hospital actually incurs (after ground-truth outcomes are revealed). We plot the histogram from random train/test splits of the dataset, and observe that the true loss is generally much greater than the predicted loss. Because the hospital might incur loss it didn't expect or prepare for, the hospital cannot trust the prediction function. **Right** After applying our recalibration algorithm, the true loss almost matches the predicted loss.

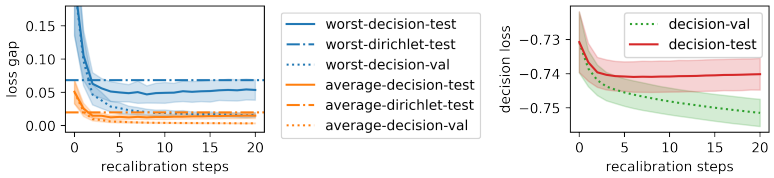

Figure 2: Calibration improves decision loss and its estimation on the HAM10000 skin legion classification dataset. **Left** The gap between the predicted decision loss and the true decision loss in Eq.(9) on a set of randomly sampled loss functions. We plot both the average gap (orange) and the worst gap (blue) out of all the loss functions. The dotted lines are the validation set performance, and solid lines are the test set performance. With more recalibration steps in Algorithm 1, both the average gap and the worst gap improves. The improvements are greater than Dirichlet recalibration (dashed line) **Right** The decision loss (averaged across all random loss functions). With more recalibration steps the decision loss also improves slightly.

the decision loss estimation error. For the estimation error, as in Definition 3 for any loss function ℓ and corresponding Bayes decision rule δ_ℓ we measure

$$\text{loss gap} := \left|\mathbb{E}[\ell(\hat{Y}, \delta_\ell(\hat{p}(X)))] - \mathbb{E}[\ell(Y, \delta_\ell(\hat{p}(X)))]\right| / \sup_{a\in\mathcal{A}} \|\ell(\cdot, a)\|_2$$

In addition to the loss function in Figure 1 (which is motivated by medical domain knowledge), we also consider a set of 500 random loss functions where for each $y \in \mathcal{Y}, a \in \mathcal{A}$, $\ell(y, a) \sim \text{Normal}(0, 1)$, and report both the average loss gap and the maximum loss gap across the loss functions.

Setup We use the HAM10000 dataset (Tschandl et al., 2018). We partition the dataset into train/validation/test sets, where approximately 15% of the data are used for validation, while 10% are used for the test set. We use the train set to learn the baseline classifier $\hat{p}$, validation set to recalibrate, and the test set to measure final performance. For modeling we use the densenet-121 architecture (Huang et al., 2017), which achieves around 90% accuracy.

Methods For our method we use Algorithm 2 in Appendix A (which is a small extension of Algorithm 1 explained in Section 4.4). We compare with temperature scaling (Guo et al., 2017) and Dirichlet calibration (Kull et al., 2019). We observe that all recalibration methods (including ours) work better if we first apply temperature scaling, hence we first apply it in all experiments. For example, in Figure 2 temperature scaling corresponds to 0 decision recalibration steps.

Results The results are shown in Figure 2. For these experiments we set the number of actions $K = 3$. For other choices we obtain qualitatively similar results in Appendix C. The main observation

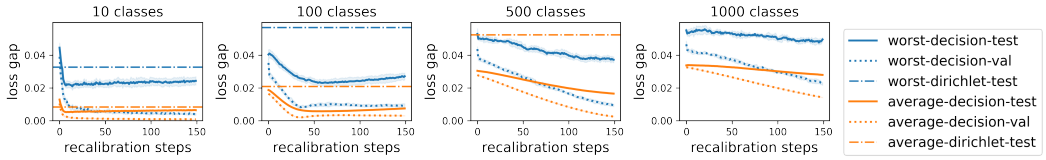

Figure 3: Calibration improves decision loss estimation on Imagenet-1000. The meaning of the plot is identical to Figure 2. From left to right we vary the number of classification categories C from 10 to 1000. Our algorithm reduces the gap between predicted loss and true loss in Eq.(9) even up to 1000 classes, although more classes require more iterations and are more prone to over-fitting. Dirichlet calibration is less scalable than our method. For example, with 1000 classes the loss gap of Dirichlet calibration is off the chart.

is that decision recalibration improves the loss gap in Eq.(9) and slightly improves the decision loss. Our recalibration algorithm converges rather quickly (in about 5 steps). We also observe that our recalibration algorithm slightly improves top-1 accuracy (the average improvement is $0.40 \pm 0.08\%$) and L2 loss (the average decrease is 0.010 ± 0.001) on the test set.

5.2 Imagenet Classification

We stress test our algorithm on Imagenet. The aim is to show that even with deeply optimized classifiers (such as inception-v3 and resnet) that are tailor made for the Imagenet benchmark and a large number of classes (1000 classes), our recalibration algorithm can improve the loss gap in Eq.(9).

Setup The setup and baselines are identical to the HAM10000 experiment with two differences: we use pretrained models provided by pytorch, and among the 50000 standard validation samples, we use 40000 samples for recalibration and 10000 samples for testing. Similar to the previous experiment, we randomly generate a set of 500 loss functions from normal distributions.

Results The results are shown in Figure 3 with additional plots in Appendix C. Decision calibration can generalize to a larger number of classes, and still provides some (albeit smaller) benefits with 1000 classes. Recalibration does not hurt accuracy and L2 error, as we observe that both improve by a modest amount (on average by 0.30% and 0.00173 respectively). We contrast decision calibration with Dirichlet calibration (Kull et al., 2019). Dirichlet calibration also reduces the loss gap when the number of classes is small (e.g. 10 classes), but is less scaleble than decision recalibration. With more classes its performance degrades much more than decision calibration.

6 Related Work

Calibration Early calibration research focus on binary classification (Brier, 1950; Dawid, 1984). For multiclass classification, the strongest definition is distribution (strong) calibration (Kull & Flach, 2015; Song et al., 2019) but is hindered by sample complexity. Weaker notions such as confidence (weak) calibration (Platt et al., 1999; Guo et al., 2017), class-wise calibration (Kull et al., 2019) or average calibration average calibration (Kuleshov et al., 2018) are more commonly used in practice. To unify these notions, (Widmann et al., 2019) proposes $\mathcal{F}$-calibration but lacks detailed guidance on which notions to use.

Individual calibration Our paper discusses the *average* decision loss over the population X. A stronger requirement is to guarantee the loss for each individual decision. Usually individual guarantees are near-impossible (Barber et al., 2019) and are only achievable with hedging (Zhao & Ermon, 2021) or randomization (Zhao et al., 2020).

Multi-calibration and Outcome Indistinguishability. Calibration have been the focus of many works on fairness, starting with (Kleinberg et al., 2016; Pleiss et al., 2017). Multi-calibration has emerged as a noteworthy notion of fairness (Hébert-Johnson et al., 2018; Kim et al., 2019; Dwork et al., 2019; Shabat et al., 2020; Jung et al., 2020; Dwork et al., 2021) because it goes beyond "protected" groups, and guarantees calibration for any group that is identifiable within some computational bound. Recently, (Dwork et al., 2021) generalizes multicalibration to outcome indistinguishability (OI). Decision calibration is a special form of OI.

7 Conclusion

We discussed why calibration is important for decision makers, and show that calibration typically implies two desiderata: no regret and accurate loss estimation. We showed that it is possible to achieve these desiderata for realistic decision makers choosing between a bounded number of actions.

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A Relaxations to Decision Calibration

We define the algorithm that corresponds to Algorithm 1 but for softmax relaxed functions. Before defining our algorithm at each iteration t we first lighten our notation with a shorthand $b_a(X) = b(\hat{p}^{(t-1)}(X), a)$ (at different iteration t, b_a denotes different functions).

Algorithm 2: Recalibration Algorithm to achieve decision calibration.

1 Input current prediction function $\hat{p}$, a dataset $\mathcal{D} = \{(x_1, y_1), \cdots, (x_M, y_M)\}$ tolerance ϵ ;
2 Initialize $\hat{p}^{(0)} = \hat{p}$;
3 **for** $t = 1, 2, \cdots$ *until* $v^{(t-1)} > \epsilon$ **do**
4 $\quad v^{(t)}, b^{(t)} = \sup, \arg\sup_{b \in \bar{B}^K} \sum_{a=1}^{K} \left\| \mathbb{E}[(Y - \hat{p}^{(t-1)}(X)) b_a(X)] \right\|$;
5 $\quad$ Compute $D \in \mathbb{R}^{K \times K}$ where $D_{aa'} = \mathbb{E}[b_a^{(t)}(X) b_{a'}^{(t)}(X)]$;
6 $\quad$ Compute $R \in \mathbb{R}^{K \times C}$ where $R_a = \mathbb{E}[(Y - \hat{p}^{t-1}(X)) b_a^{(t)}(X)]$;
7 $\quad$ Set $\hat{p}^{(t)} : x \mapsto \pi(\hat{p}^{(t-1)}(x) + R^T D^{-1} b^{(t)}(x))$ where π is the normalization projection;
8 **end**
9 Output $\hat{p}^{(T)}$ where T is the number of iterations

For the intuition of the algorithm, consider the t-th iteration where the current prediction function is $\hat{p}^{(t-1)}$. The objective of line 5-6 is to compute the adjustments $U \in \mathbb{R}^{C \times K}$ such that

$$\hat{p}^{(t)}(X) = \hat{p}^{(t-1)}(X) + U b^{(t)}(X)$$

can minimize

$$L(U) := \sum_{a=1}^{K} \left\| \mathbb{E}[(Y - \hat{p}^{(t)}(X)) b_a^{(t)}(X)] \right\|^2$$

Intuitively, we find the worst case b that maximizes the "error" $\sum_{a=1}^{K} \left\| \mathbb{E}[(Y - \hat{p}^{t-1}(X)) b_a^{(t)}(X)] \right\|^2$, and we make the adjustment to minimize this error. We make some simple algebraic manipulations on L to get

$$\begin{aligned} L(U) &= \sum_{a=1}^{K} \left\| \mathbb{E}[(Y - \hat{p}^{(t-1)}(X)) b_a^{(t)}(X) - U b^{(t)}(X) b_a^{(t)}(X)] \right\|^2 \\ &= \sum_{a=1}^{K} \left\| R_a - (DU^T)_a \right\|^2 = \left\| R - DU^T \right\|^2 \end{aligned}$$

Suppose D is invertible, then the optimum of the objective is

$$U^* := \arg\inf L(U) = R^T D^{-1}, \quad L(U^*) = 0$$

For the relaxed algorithm we also have a theorem that is equivalent to Theorem 2.2. The statement of the theorem is identical; the proof is also essentially the same except for the use of some new technical tools.

Theorem 2.2'. *Algorithm 2 terminates in $O(1/\epsilon^2)$ iterations. Given $O(poly(K, C, \log(1/\delta)))$ samples, with $1 - \delta$ probability Algorithm 1 outputs a $(\mathcal{L}^K, \epsilon)$-decision calibrated prediction function $\hat{p}'$ that satisfies $\mathbb{E}[\|\hat{p}'(X) - Y\|_2^2] \leq \mathbb{E}[\|\hat{p}(X) - Y\|_2^2]$.*

B Decision Calibration over a Bounded Action Space

As we've seen, in full generality, distribution calibration requires decision calibration over an action space that can grow exponentially in the number of classes C, but this is both difficult and unnecessary. This growing action space, however, is predicated on the support size of the predictor. We show, somewhat surprisingly, that $\mathcal{L}^K$-decision calibration implies an on-average version of distribution calibration, with no increase in loss for any bounded-action decision-maker.

Theorem 3. *Suppose $\hat{p}$ is $\mathcal{L}^K$-decision calibrated. Then, for any loss function $\ell \in \mathcal{L}^K$, we can construct a predictor $\hat{p}_\ell$ of support size $\leq K$, such that:*

- *$\hat{p}_\ell$ is distribution calibrated*
- *the optimal decision rule is preserved $\delta_\ell(\hat{p}_\ell(x)) = \delta_\ell(\hat{p}(x))$ for all $x \in \mathcal{X}$; thus, $\mathbb{E}[\ell(Y, \delta_\ell(\hat{p}_\ell(X)))] = \mathbb{E}[\ell(Y, \delta_\ell(\hat{p}(X)))]$.*

In other words, for any decision-maker that has a loss $\ell \in \mathcal{L}^K$, an $\mathcal{L}^K$-decision calibrated predictor $\hat{p}$ is effectively distribution calibrated: the decision rule that arises from $\hat{p}$ also arises from an equally-informative predictor that is distribution calibrated. Importantly, the guarantee holds simultaneously for all $\ell \in \mathcal{L}^K$. Thus, if the ML service learns an $\mathcal{L}^K$-decision calibrated predictor, they can provide it to any bounded-action decision-maker with a guarantee akin to that of distribution calibration.

This result may seem counterintuitive; after all, we have already argued that reasoning about distribution calibration may be statistically infeasible, but have shown a statistically feasible algorithm for achieving (approximate) $\mathcal{L}^K$-decision calibration. The key point is that the distribution calibrated predictors that arise from this construction have bounded support. This allows us to sidestep the information-theoretic lower bounds, which rely on large support predictors. The intuition behind the argument is highlighted in the following Lemma (which is a direct consequence of Eq.(14) in the proof of Prosition 3.

Lemma 1. *A predictor $\hat{p}$ is $\mathcal{L}^K$-decision calibrated if and only if for all $a \in [K]$,*

$$\mathbb{E}_X \mathbb{E}_{\hat{Y} \sim \hat{p}(X)}[\hat{Y} \mid \delta_\ell(\hat{p}(X)) = a] = \mathbb{E}_X \mathbb{E}_{Y \sim p^*(X)}[Y \mid \delta_\ell(\hat{p}(X)) = a]$$

In this sense, calibrating predictions to decisions gives a pathway to achieving a strong notion of calibration without an exponential dependence on the number of classes.

With this lemma in place, we show that a simple compression scheme achieves the properties required for Theorem 3. Given a loss $\ell \in \mathcal{L}^K$, we compress the predictions along the partitions defined by δ_ℓ.

Proof of Theorem 3. Suppose $\hat{p}$ is $\mathcal{L}^K$-decision calibrated. For a fixed loss $\ell \in \mathcal{L}^K$, consider the following predictor $\hat{p}_\ell$ that arises by compressing $\hat{p}$ according to the optimal decision rule δ_ℓ.

$$\hat{p}_\ell(x) = \mathbb{E}_X[\hat{p}(X) \mid \delta_\ell(\hat{p}(X)) = \delta_\ell(\hat{p}(x))]$$

First, note that by averaging over each set, the support size of $\hat{p}_\ell$ is bounded by at most K. Next, we note that by construction and Lemma 1, $\hat{p}_\ell$ is distribution calibrated. To see this, consider each $q \in \Delta^C$ supported by $\hat{p}_\ell$; for each q, there is some optimal action $a_q \in [K]$. That is, the sets $\{x : \hat{p}_\ell(x) = q\} = \{x : \delta_\ell(\hat{p}(x)) = a_q\}$ are the same. Distribution calibration follows.

$$\begin{aligned}
\mathbb{E}_X \mathbb{E}_{Y \sim p^*(X)}[Y \mid \hat{p}_\ell(X) = q] &= \mathbb{E}_X \mathbb{E}_{Y \sim p^*(X)}[Y \mid \delta_\ell(\hat{p}(X)) = a_q] \\
&= \mathbb{E}_X \mathbb{E}_{\hat{Y} \sim \hat{p}_\ell(X)}[\hat{Y} \mid \delta_\ell(\hat{p}(X)) = a_q] \\
&= \mathbb{E}_X \mathbb{E}_{\hat{Y} \sim \hat{p}_\ell(X)}[\hat{Y} \mid \hat{p}_\ell(X) = q] \\
&= q
\end{aligned}$$

Finally, it remains to show that the optimal decision rule resulting from $\hat{p}_\ell$ and $\hat{p}$ are the same, pointwise for all $x \in \mathcal{X}$. As an immediate corollary, the expected loss using $\hat{p}_\ell$ and $\hat{p}$ is the same. We show that the decision rule will be preserved by the fact that for each $x \in \mathcal{X}$, the compressed prediction is a convex combination of predictions that gave rise to the same optimal action.

Specifically, consider any x such that $\hat{p}_\ell(x) = q$. By the argument above, there is some action $a_q \in [K]$ that is optimal for all such x. Optimality implies that for all $a \in [K]$

$$\langle \ell_{a_q}, \hat{p}(x) \rangle \leq \langle \ell_a, \hat{p}(x) \rangle.$$

Thus, by linearity of expectation, averaging over $\{x : \hat{p}_\ell(x) = q\}$, the optimal action a_q is preserved.

$$\begin{aligned}
\langle \ell_{a_q}, q \rangle &= \langle \ell_{a_q}, \mathbb{E}[\hat{p}(X) \mid \delta_\ell(\hat{p}(X)) = a_q] \rangle \\
&= \mathbb{E}[\langle \ell_{a_q}, \hat{p}(X) \rangle \mid \delta_\ell(\hat{p}(X)) = a_q] \\
&\leq \mathbb{E}[\langle \ell_a, \hat{p}(X) \rangle \mid \delta_\ell(\hat{p}(X)) = a_q] \\
&= \langle \ell_a, \mathbb{E}[\hat{p}(X) \mid \delta_\ell(\hat{p}(X)) = a_q] \rangle \\
&= \langle \ell_a, q \rangle
\end{aligned}$$

Thus, the optimal action is preserved for all $x \in \mathcal{X}$. □

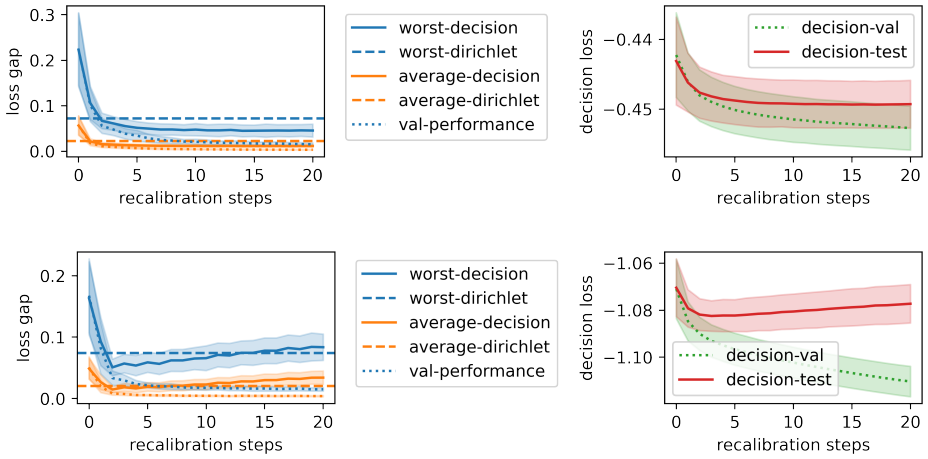

Figure 4: Additional Results on the HAM10000 for 2 and 5 actions. The observations are similar to Figure 2 even though overfitting happens sooner with 5 actions

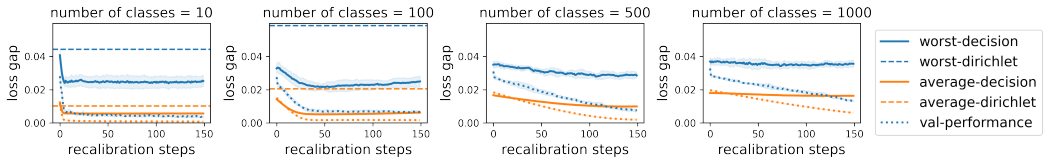

Figure 5: Additional results on the resnet18. The observations are similar to Figure 3: decision recalibration improves the loss gap.

We note that this proof shows a tight implication of distribution calibration given exact $\mathcal{L}^K$-decision calibration. A similar argument shows that approximate $\mathcal{L}^K$-decision calibration implies an on-average relaxation of distribution calibration. That is, rather than a guarantee that conditions on $\delta_\ell(\hat{p}(X)) = q$, we can give a guarantee on the joint distribution over Y and $\delta_\ell(\hat{p}(X))$. In particular, the relative calibration error incurred on actions of small density (i.e., those $a \in [K]$ such that the probability that $\delta_\ell(\hat{p}(X)) = a$ is small but not 0) may be large, simply because they are rare events.

C Additional Experiment Details and Results

Additional experiments are shown in Figure 4 and Figure 5. The observations are similar to those in the main paper.

D Proofs

D.1 Equivalence between Decision Calibration and Existing Notions of Calibration

Proof of Theorem 1, part 1. Before the proof we first need a technical Lemma

Lemma 2. *For any pair of random variables U, V, $\mathbb{E}[U \mid V] = 0$ almost surely if and only if $\forall c \in \mathbb{R}, \mathbb{E}[U\mathbb{I}(V > c)] = 0$.*

Part 1 When the loss function is $\ell : y, a \mapsto \mathbb{I}(y \neq a \cap a \neq \perp) + \beta\mathbb{I}(a = \perp)$, the Bayes decision is given by

$$\delta_\ell(x) = \begin{cases} \arg\max \hat{p}(x) & \max \hat{p}(x) > 1 - \beta \\ \perp & \text{otherwise} \end{cases}$$

Denote $U = \max \hat{p}(X)$ and $V = \arg\max \hat{p}(X)$. For any pair of loss functions ℓ and ℓ' parameterized by β and β' we have

$$\begin{aligned}
&\mathbb{E}[\ell'(Y, \delta_\ell(X))] - \mathbb{E}[\ell'(\hat{Y}, \delta_\ell(X))] \\
&= \mathbb{E}[(\ell'(Y, \perp) - \ell'(\hat{Y}, \perp))\mathbb{I}(\delta_\ell(X) = \perp)] + \mathbb{E}[(\ell'(Y, \delta_\ell(X)) - \ell'(\hat{Y}, \delta_\ell(X)))\mathbb{I}(\delta_\ell(X) \neq \perp)] && \text{Tower} \\
&= 0 + \mathbb{E}[(p^*_V(X) - \hat{p}_V(X))\mathbb{I}(\max \hat{p}(x) > 1 - \beta)] && \text{Def of } \ell \\
&= \mathbb{E}[(p^*_V - U)\mathbb{I}(U > 1 - \beta)]
\end{aligned}$$

Suppose $\hat{p}$ is confidence calibrated, then almost surely

$$U = \Pr[Y = \arg\max \hat{p}(X) \mid U] = \mathbb{E}[p^*_V(X) \mid U]$$

which implies almost surely $\mathbb{E}[p^*_V(X) - U \mid U] = 0$. By Lemma 1 we can conclude that

$$0 = \mathbb{E}[(p^*_V(X) - U)\mathbb{I}(U > 1 - \beta)] = \mathbb{E}[\ell(Y, \delta^*(X))] - \mathbb{E}[\ell(\hat{Y}, \delta^*(X))]$$

so $\hat{p}$ is L_r-weakly calibrated.

Conversely suppose $\hat{p}$ is L_r weakly calibrated, then $\forall \beta > \mathbb{R}$, $\mathbb{E}[(p^*_V(X) - U)\mathbb{I}(U > 1 - \beta)] = 0$. By Lemma 1 we can conclude that almost surely

$$0 = \mathbb{E}[p^*_V(X) - U \mid U] = \mathbb{E}[p^*_V(X) \mid U] - U$$

so $\hat{p}$ is confidence calibrated.

Part 2 For any loss function $\ell : y, a \mapsto \mathbb{I}(a = \perp) + \beta_1\mathbb{I}(y \neq c, a = T) + \beta_2\mathbb{I}(y = c, a = F)$ where $\beta_1, \beta_2 > 1$, observe that the Bayes decision for loss function ℓ is

$$\delta^*(x) = \begin{cases} T & \hat{p}_c(x) > \max(1 - 1/\beta_1, \beta_1/(\beta_1 + \beta_2)) \\ F & \hat{p}_c(x) < \min(1/\beta_2, \beta_1/(\beta_1 + \beta_2)) \\ \perp & \text{otherwise} \end{cases}$$

Note that we can choose β_1, β_2 to obtain any threshold $\alpha := \max(1 - 1/\beta_1, \beta_1/(\beta_1 + \beta_2)), \gamma := \min(1/\beta_2, \beta_1/(\beta_1 + \beta_2))$. For any pair of loss functions ℓ and ℓ' parameterized by $\beta_1, \beta_2, \beta'_1, \beta'_2$ (with associated threshold $\alpha \geq \gamma, \alpha' \geq \gamma'$) we have

$$\begin{aligned}
&\mathbb{E}[\ell'(Y, \delta_\ell(X)) - \mathbb{E}[\ell'(\hat{Y}, \delta_\ell(X))] \\
&= \mathbb{E}[(\ell'('Y, \delta_\ell(X)) - \ell'(\hat{Y}, \delta_\ell(X)))\mathbb{I}(\delta_\ell = T)] + \mathbb{E}[(\ell'(Y, \delta_\ell(X)) - \ell'(\hat{Y}, \delta_\ell(X)))\mathbb{I}(\delta_\ell = F)] \\
&= \mathbb{E}[(p^*_c(X) - \hat{p}_c(X))\mathbb{I}(\hat{p}_c(X) > \alpha)] + \mathbb{E}[(p^*_c(X) - \hat{p}_c(X))\mathbb{I}(\hat{p}_c(X) < \gamma)]
\end{aligned}$$

Similar to the argument for part 2, the predictor $\hat{p}$ is classwise calibrated if and only if $\mathbb{E}[(p^*_c(X) - \hat{p}_c(X))\mathbb{I}(\hat{p}_c(X) > \alpha)]$; $\hat{p}$ is classwise calibrated if and only if $\mathbb{I}(\hat{p}_c(X) > \alpha)] + \mathbb{E}[(p^*_c(X) - \hat{p}_c(X))\mathbb{I}(\hat{p}_c(X) < \gamma)]$; therefore it is classwise calibrated if and only if it is $\mathcal{L}_{cr}$-decision calibrated.

Part 3 Choose the special loss function $\mathcal{A} = \Delta^C$ and ℓ as the log loss $\ell : y, a \mapsto \log a_y$ then the Bayes action can be computed as

$$\delta_\ell(x) = \arg \inf_{a \in \Delta^C} \mathbb{E}_{\hat{Y} \sim \hat{p}(X)}[\log a_{\hat{Y}}] = \hat{p}(x)$$

Denote $U = \hat{p}(X)$ then let $\mathcal{L}_B$ be the set of all bounded loss functions, i.e. $\mathcal{L}_B = \{\ell, |\ell(y, a)| \leq B\}$

$$\begin{aligned}
&\sup_{\ell' \in \mathcal{L}_B} \mathbb{E}[\ell'(Y, \delta_\ell(X))] - \mathbb{E}[\ell'(\hat{Y}, \delta_\ell(X))] \\
&\sup_{\ell' \in \mathcal{L}_B} \mathbb{E}[\mathbb{E}[\ell'(Y, U) - \ell'(\hat{Y}, U) \mid U]] && \text{Tower} \\
&= \frac{1}{B}\mathbb{E}[\|\mathbb{E}[p^*(X) - \hat{p}(X) \mid U]\|_1] && \text{Cauchy Schwarz}
\end{aligned}$$

If $\hat{p}$ satisfies distribution calibration, then $\|\mathbb{E}[p^*(X) - \hat{p}(X) \mid U]\|_1 = 0$ almost surely, which implies that $\hat{p}$ is $\mathcal{L}_B$ decision calibrated. Conversely, if $\hat{p}$ is $\mathcal{L}_B$ decision calibrated, then $\|\mathbb{E}[p^*(X) - \hat{p}(X) \mid U]\|_1 = 0$ almost surely (because if the expectation of a non-negative random variable is zero, the random variable must be zero almost surely). The Theorem follows because B is arbitrarily chosen. □

D.2 Proofs for Section 4

Proposition 3. *$\hat{p}$ satisfies $(\mathcal{L}^K, \epsilon)$-decision calibration if and only if*

$$\sup_{b \in B^K} \sum_{a=1}^{K} \left\| \mathbb{E}[(\hat{Y} - Y) b(\hat{p}(X), a)] \right\|_2 \leq \epsilon$$

Proof of Proposition 3. Because $\mathcal{A} = [K]$ and $\mathcal{Y} \simeq [C]$, a loss function can be uniquely identified with K vectors $\ell_1, \cdots, \ell_K$ where $\ell_{ac} = \ell(c, a)$. Given prediction function $\hat{p} : \mathcal{X} \to \Delta^C$ and the expected loss can be denoted as

$$\mathbb{E}_{\hat{Y} \sim \hat{p}(x)}[\ell(\hat{Y}, a)] = \langle \hat{p}(x), \ell_a \rangle \tag{9}$$

Choose any Bayes decision function $\delta_{\ell'}$ for some loss $\ell' \in \mathcal{L}^K$, as a notation shorthand denote $\delta_{\ell'}(\hat{p}(x)) = \delta_{\ell'}(x)$. We can compute the gap between the left hand side and right hand side of Definition 2 as

$$= \sup_{\ell, |\ell(\cdot,a)|_2 \leq 1} \left| \mathbb{E}_{X \sim p^*_X, \hat{Y} \sim \hat{p}(X)}[\ell(\hat{Y}, \delta(\hat{p}(X)))] - \mathbb{E}_{X \sim p^*_X, Y \sim p^*(X)}[\ell(Y, \delta(\hat{p}(X)))] \right| \tag{10}$$

$$= \sup_{\ell, |\ell(\cdot,a)|_2 \leq 1} \left| \mathbb{E}\left[\langle \ell_{\delta_{\ell'}(X)}, \hat{p}(X) \rangle \right] - \mathbb{E}\left[\langle \ell_{\delta_{\ell'}(X)}, p^*(X) \rangle \right] \right| \tag{11}$$

$$= \sup_{\ell, |\ell(\cdot,a)|_2 \leq 1} \left| \sum_a \mathbb{E}[\langle \hat{p}(X), \ell_a \rangle \mathbb{I}(\delta_{\ell'}(X) = a)] - \sum_a \mathbb{E}[\langle \hat{p}(X), \ell_a \rangle \mathbb{I}(\delta_{\ell'}(X) = a)] \right| \tag{12}$$

$$= \sup_{\ell, |\ell(\cdot,a)|_2 \leq 1} \left| \sum_a \langle \mathbb{E}[(p^*(X) - \hat{p}(X)) \mathbb{I}(\delta_{\ell'}(X) = a)], \ell_a \rangle \right| \quad \text{Linearity} \tag{13}$$

$$= \sum_a \| \mathbb{E}[(p^*(X) - \hat{p}(X)) \mathbb{I}(\delta_{\ell'}(X) = a)] \|_* \quad \text{Cauchy Schwarz} \tag{14}$$

Finally we complete the proof by observing that the set of maps

$$\{q, a \mapsto \mathbb{I}(\delta_\ell(q) = a), \ell \in \mathcal{L}^K\}$$

is the same as the set of maps B^K. We do this by establishing a one-to-one correspondence where $\ell_a = -w_a / \|w_a\|_2$ then

$$\mathbb{I}(\delta_\ell(q) = a) = \mathbb{I}(\arg\inf_{a'} \langle \ell_{a'}, q \rangle = a) = \mathbb{I}(\arg\sup_{a'} \langle w_{a'}, q \rangle = a)$$

□

Formal Statement of Theorem 2, part I . We first define a new notation. Given a set of samples $\mathcal{D} = \{(X_1, Y_1), \cdots, (X_N, Y_N)\}$, denote $\hat{\mathbb{E}}_{\mathcal{D}}[\psi(X, Y)]$ as the empirical expectation, i.e.

$$\hat{\mathbb{E}}_{\mathcal{D}}[\psi(X, Y)] := \frac{1}{N} \sum_n \psi(X_n, Y_n)$$

Theorem 2.1 (Formal)**.** *Let B^K be as defined by Eq.(5), for any true distribution over X, Y and any $\hat{p}$, given a set of N samples $\mathcal{D} = \{(X_1, Y_1), \cdots, (X_N, Y_N)\}$, with probability $1 - \delta$ over random draws of $\mathcal{D}$,*

$$\sup_{b \in B^K} \sum_{a=1}^{K} \| \mathbb{E}[(\hat{p}(X) - Y) b(\hat{p}(X), a)] \|_2 - \sum_{a=1}^{K} \left\| \hat{\mathbb{E}}_{\mathcal{D}}[(\hat{p}(X) - Y) b(\hat{p}(X), a)] \right\|_2 \leq \tilde{O}\left(\frac{K^{3/2} C}{\sqrt{N}} \right) \tag{15}$$

where $\tilde{O}$ denotes equal up to constant and logarithmic terms.

Proof of Theorem 2.1. Before proving this theorem we first need a few uniform convergence Lemmas which we will prove in Appendix D.3.

Lemma 3. *Let B by any set of functions $\{b : \Delta^C \to [0,1]\}$ and U, V be any pair of random variables where U takes values in $[-1,1]^C$ and V takes values in Δ^C. Let $\mathcal{D} = \{(U_1, V_1), \cdots, (U_N, V_N)\}$ be an i.i.d. draw of N samples from U, V, define the Radamacher complexity by*

$$\mathcal{R}_N(B) := \mathbb{E}_{\mathcal{D}}\left[\sup_{b\in B} \frac{1}{N}\sum_{n=1}^{N} \sigma_i b(V_i)\right]$$

then for any $\delta > 0$, with probability $1-\delta$ (under random draws of $\mathcal{D}$), $\forall b \in B$

$$\|\hat{\mathbb{E}}_{\mathcal{D}}[Ub(V)] - \mathbb{E}[Ub(V)]\|_2 \le \sqrt{C}\mathcal{R}_N(B) + \sqrt{\frac{2}{N}\log\frac{2C}{\delta}}$$

Lemma 4. *Define the function family*

$$B_a^K = \left\{ b : z \mapsto \mathbb{I}(a = \arg\sup_{a'} \langle z, w_a\rangle), , w_a \in \mathbb{R}^C, a = 1, \cdots, K, z \in \Delta^C \right\}$$
$$\bar{B}_a^K = \left\{ b : z \mapsto \frac{e^{\langle z, w_a\rangle}}{\sum_{a'} e^{\langle z, w_{a'}\rangle}}, w_a \in \mathbb{R}^C, a = 1, \cdots, K, z \in \Delta^C \right\}$$

then the Radamacher complexity can be upper bounded by

$$\mathcal{R}_N(B_a^K) = O\left(\sqrt{\frac{CK\log K\log N}{N}}\right)$$
$$\mathcal{R}_N(\bar{B}_a^K) = O\left(\left(\frac{K}{N}\right)^{1/4}\log\frac{N}{K}\right)$$

As a notation shorthand denote $U = \hat{p}(X) - Y$. Note that U is a random vector raking values in $[-1,1]^N$. We can rewrite the left hand side of Eq.(15) as

$$\sup_{b\in B^K}\sum_a \|\hat{\mathbb{E}}_{\mathcal{D}}[Ub(\hat{p}(X), a)]\|_2 - \|\mathbb{E}[Ub(\hat{p}(X), a)]\|_2 \tag{16}$$
$$\le \sum_a \sup_{b\in B_a^K} \|\hat{\mathbb{E}}_{\mathcal{D}}[Ub(\hat{p}(X), a)]\|_2 - \|\mathbb{E}[Ub(\hat{p}(X), a)]\|_2 \quad \text{Jensen} \tag{17}$$
$$\le \sum_a \sup_{b\in B_a^K} \|\hat{\mathbb{E}}_{\mathcal{D}}[Ub(\hat{p}(X), a)] - \mathbb{E}[Ub(\hat{p}(X), a)]\|_2 \quad \text{Triangle} \tag{18}$$
$$\le \sum_a \sqrt{C}\mathcal{R}_N(B^K) + \sqrt{\frac{2}{N}\log\frac{2C}{\delta}} \quad \text{Lemma 3} \tag{19}$$
$$\le \sum_a \sqrt{C}O\left(\sqrt{\frac{CK\log K\log N}{N}}\right) + \sqrt{\frac{2}{N}\log\frac{2C}{\delta}} \quad \text{Lemma 4} \tag{20}$$
$$\le K\sqrt{C}O\left(\sqrt{\frac{CK\log K\log N}{N}}\right) + K\sqrt{\frac{2}{N}\log\frac{2C}{\delta}} \tag{21}$$
$$= \tilde{O}\left(\frac{K^{3/2}C}{\sqrt{N}}\right) \tag{22}$$

□

Formal Statement Theorem 2, Part II

Theorem 2.2 (Formal)**.** *Algorithm 1 terminates in $O(1/\epsilon^2)$ iterations. Given $O(poly(K, C, \log(1/\delta)))$ samples, with $1-\delta$ probability Algorithm 1 outputs a $(\mathcal{L}^K, \epsilon)$-decision calibrated prediction function $\hat{p}'$ that satisfies $\mathbb{E}[\|\hat{p}'(X) - Y\|_2^2] \le \mathbb{E}[\|\hat{p}(X) - Y\|_2^2]$.*

Proof of Theorem 2.2. We adapt the proof strategy in (Hébert-Johnson et al., 2018). The key idea is to show that a potential function must decrease after each iteration of the algorithm. We choose the potential function as $\mathbb{E}[(Y - \hat{p}(X))^2]$. Suppose at iteration k we have found a b

$$\sum_a \|\mathbb{E}[(\hat{p}(X) - Y)b(X, a)]\|^2 \geq \epsilon^2 \tag{23}$$

Denote $\gamma \in \mathbb{R}^{K \times K}$ where $\gamma_a = \mathbb{E}[(Y - \hat{p}(X))b(X, a)] + e_a$ where e_a is the estimation error. From Lemma 3 and Lemma 4 we can observe that with polynomial samples $\sum_a \|e_a\|^2 \leq \epsilon^2/2$. The adjustment we make is $\hat{p}'(X) = \pi(\hat{p}(X) + \sum_a \gamma_a b(X, a))$

$$\mathbb{E}[\|Y - \hat{p}(X)\|^2] - \mathbb{E}[\|Y - \hat{p}'(X)\|^2] \tag{24}$$

$$= \mathbb{E}[\|Y - \hat{p}(X)\|^2 - \|Y - \pi(\hat{p}(X) + \sum_a \gamma_a b(X, a) + e_a)\|^2] \tag{25}$$

$$= \mathbb{E}[\|Y - \hat{p}(X)\|^2 - \|Y - \hat{p}(X) + \sum_a \gamma_a b(X, a) + e_a\|^2] \quad \text{Projection} \tag{26}$$

$$= \mathbb{E}[\|Y - \hat{p}(X)\|^2 - \|Y - \hat{p}(X) - \sum_a \gamma_a b(X, a)\|^2 \tag{27}$$

$$+ \|e_a\|^2 - 2(Y - \hat{p}(X) - \sum_a \gamma_a b(X, a))^T e_a] \tag{28}$$

$$\geq \mathbb{E}[\|Y - \hat{p}(X)\|^2 - \|Y - \hat{p}(X) - \sum_a \gamma_a b(X, a)\|^2 \tag{29}$$

$$+ \|e_a\|^2 - 2(Y - \hat{p}(X) - \sum_a \gamma_a b(X, a))^T e_a] \tag{30}$$

$$\geq \mathbb{E}\left[(2Y - 2\hat{p}(X) - \sum_a \gamma_a b(X, a))^T \left(\sum_a \gamma_a b(X, a)\right)\right] - \epsilon^2/2 \tag{31}$$

$$= \mathbb{E}\left[\sum_a \gamma_a^T b(X, a)(2Y - 2\hat{p}(X)) - \left\|\sum_a \gamma_a b(X, a)\right\|^2\right] - \epsilon^2/2 \tag{32}$$

$$= \mathbb{E}\left[2\sum_a \|\gamma_a\|^2 - \left\|\sum_a \gamma_a b(X, a)\right\|^2\right] - \epsilon^2/2 \tag{33}$$

$$\geq \sum_a \|\gamma_a\|^2 - \epsilon^2/2 \geq \epsilon^2/2 \quad \text{Jensen} \tag{34}$$

$$\tag{35}$$

Because initially $\mathbb{E}[\|p^*(X) - \hat{p}(X)\|^2] \leq \sqrt{2}$ the algorithm must converge in $2\sqrt{2}/\epsilon^2$ iterations. □

Proof of Theorem 2.2'. Observe that the matrix D defined in Algorithm 2 is a symmetric, positive semi-definite and non-negative matrix such that $\sum_{a,a'} D_{aa'} = 1$. To show that the algorithm converges we first need two Lemmas on the properties of such matrices. For a positive semi-definite (PSD) symmetric matrix, let λ_1 denote the largest eigenvalue, and λ_n denote the smallest eigenvalue. The first Lemma is a simple consequence of the Perron-Frobenius theorem,

Lemma 5. *Let D be any symmetric PSD non-negative matrix such that $\sum_{a,a'} D_{aa'} = 1$, then $\lambda_1(D) \leq 1$, so $\lambda_n(D^{-1}) \geq 1$.*

Lemma 6 ((Fang et al., 1994) Theorem 1)**.** *Let D be a symmtric PSD matrix, then for any matrix B (that can multiply with D)*

$$\lambda_n(D)\text{trace}(B) \leq \text{trace}(BD) \leq \lambda_1(D)\text{trace}(B)$$

Now we can proveed to prove our main result. We have to show that the L2 error $\mathbb{E}[(Y - \hat{p}^{(t-1)}(X))^2]$ must decrease at iteration t if we still have

$$\epsilon^2 \leq \sum_a \|\mathbb{E}[(Y - \hat{p}^{(t-1)})b_a^{(t)}]\|^2 := \text{trace}(RR^T)$$

We can compute the reduction in L2 error after the adjustment

$$
\begin{aligned}
&\mathbb{E}[(Y-\hat{p}^{(t-1)}(X))^2]-\mathbb{E}[(Y-\hat{p}^{(t)}(X))^2] \\
&=\mathbb{E}\left[(2(Y-\hat{p}^{(t-1)}(X))-R^TD^{-1}b^{(t)}(X))^TR^TD^{-1}b^{(t)}(X)\right] \\
&=2\mathbb{E}\left[(Y-\hat{p}^{(t-1)}(X))^TR^TD^{-1}b^{(t)}(X)\right]-\mathbb{E}\left[b^{(t)}(X)^TD^{-T}RR^TD^{-1}b^{(t)}(X)\right] \\
&=2\mathrm{trace}\left(\mathbb{E}\left[b^{(t)}(X)(Y-\hat{p}^{(t-1)}(X))^TR^TD^{-1}\right]\right) \\
&\quad-\mathrm{trace}\left(\mathbb{E}\left[b^{(t)}(X)b^{(t)}(X)^TD^{-T}RR^TD^{-1}\right]\right) && \text{Cyclic property} \\
&=2\mathrm{trace}\left(RR^TD^{-1}\right)-\mathrm{trace}(RR^TD^{-1})=\mathrm{trace}(RR^TD^{-1}) \\
&\geq \mathrm{trace}(RR^T)\geq\epsilon^2 && \text{Lemma 6 and 5}
\end{aligned}
$$

Therefore, the algorithm cannot run for more than $O(1/\epsilon^2)$ iterations. □

D.3 Proof of Remaining Lemmas

Proof of Lemma 2. By the orthogonal property of the condition expectation, for any event A in the sigma algebra induced by V, we have

$$\mathbb{E}[(U-\mathbb{E}[U\mid V])\mathbb{I}_A]=0$$

This includes the event $V>c$

$$\mathbb{E}[(U-\mathbb{E}[U\mid V])\mathbb{I}(V>c)]=0$$

In other words,

$$\mathbb{E}[U\mathbb{I}(V>c)]=\mathbb{E}[\mathbb{E}[U\mid V]\mathbb{I}(V>c)]$$

□

Proof of Lemma 3. First observe that by the norm inequality $\|z\|_\alpha\leq C^{1/\alpha}\|z\|_\infty$ we have

$$\|\hat{\mathbb{E}}_{\mathcal{D}}[Ub(V)]-\mathbb{E}[Ub(V)]\|_2\leq\sqrt{C}\|\hat{\mathbb{E}}[Ub(V)]-\mathbb{E}[Ub(V)]\|_\infty \tag{36}$$

Denote the c-th dimension of U by U^c; we now provide bounds for $|\hat{\mathbb{E}}[U^cb(V)]-\mathbb{E}[U^cb(V)]|$ by standard Radamacher complexity arguments. Define a set of ghost samples $\bar{\mathcal{D}}=\{(\bar{U}_1,\bar{V}_1),\cdots(\bar{U}_N,\bar{V}_N)\}$ and Radamacher variables $\sigma_n\in\{-1,1\}$

$$
\begin{aligned}
&\mathbb{E}_{\mathcal{D}}\left[\sup_b|\hat{\mathbb{E}}_{\mathcal{D}}[U^cb(V)]-\mathbb{E}[U^cb(V)]|\right] && (37)\\
&=\mathbb{E}_{\mathcal{D}}\left[\sup_b\left|\hat{\mathbb{E}}_{\mathcal{D}}[U^cb(V)]-\mathbb{E}_{\bar{\mathcal{D}}}\left[\hat{\mathbb{E}}_{\bar{\mathcal{D}}}[U^cb(V)]\right]\right|\right] && \text{Tower} \quad (38)\\
&=\mathbb{E}_{\mathcal{D}}\left[\sup_b\left|\mathbb{E}_{\bar{\mathcal{D}}}[\hat{\mathbb{E}}_{\mathcal{D}}[U^cb(V)]-\hat{\mathbb{E}}_{\bar{\mathcal{D}}}[U^cb(V)]\mid\mathcal{D}]\right|\right] && \text{Linearity} \quad (39)\\
&\leq\mathbb{E}_{\mathcal{D}}\left[\sup_b\mathbb{E}_{\bar{\mathcal{D}}}\left[\left|\hat{\mathbb{E}}_{\mathcal{D}}[U^cb(V)]-\hat{\mathbb{E}}_{\bar{\mathcal{D}}}[U^cb(V)]\right|\mid\mathcal{D}\right]\right] && \text{Jensen} \quad (40)\\
&\leq\mathbb{E}_{\mathcal{D},\bar{\mathcal{D}}}\left[\sup_b\left|\hat{\mathbb{E}}_{\mathcal{D}}[U^cb(V)]-\hat{\mathbb{E}}_{\bar{\mathcal{D}}}[U^cb(V)]\right|\right] && \text{Jensen} \quad (41)\\
&\leq\mathbb{E}_{\sigma,\mathcal{D},\bar{\mathcal{D}}}\left[\sup_b\left|\frac{1}{N}\sum_i\sigma_iU_i^cb(V_i)-\frac{1}{N}\sum_i\sigma_i\bar{U}_i^cb(\bar{V}_i)\right|\right] && \text{Radamacher} \quad (42)\\
&\leq\mathbb{E}_{\sigma,\mathcal{D},\bar{\mathcal{D}}}\left[\sup_b\left|\frac{1}{N}\sum_i\sigma_iU_i^cb(V_i)\right|+\sup_b\left|\frac{1}{N}\sum_i\sigma_i\bar{U}_i^cb(\bar{V}_i)\right|\right] && \text{Jensen} \quad (43)\\
&=2\mathbb{E}_{\sigma,\mathcal{D}}\left[\sup_b\left|\frac{1}{N}\sum_i\sigma_iU_i^cb(V_i)\right|\right] && (44)
\end{aligned}
$$

Suppose we know the Radamacher complexity of the function family b

$$\mathcal{R}_N(B) := \mathbb{E}\left[\sup_b \frac{1}{N}\sum_i \sigma_i b(V_i)\right] \tag{45}$$

Then by the contraction inequality, and observe that $U_i^c \in [-1,1]$ so multiplication by U_i^c is a 1-Lipschitz map, we can conclude for any $c \in [C]$

$$\mathcal{R}_N(B) \geq \mathbb{E}\left[\sup_b \frac{1}{N}\sum_i \sigma_i U_{ic} b(V_i)\right] \tag{46}$$

Finally observe that the map $\mathcal{D} \to \frac{1}{N}\sum_i \sigma_i U_{ic} b(V_i)$ has $2/N$ bounded difference, so by Mcdiamid inequality for any $\epsilon > 0$

$$\Pr\left[\sup_b \left|\frac{1}{N}\sum_i \sigma_i U_i^c b(V_i)\right| \geq \mathcal{R}_N(B) + \epsilon\right] \leq 2e^{-N\epsilon^2/2} \tag{47}$$

By union bound we have

$$\Pr\left[\max_c \sup_b \left|\frac{1}{N}\sum_i \sigma_i U_i^c b(V_i)\right| \geq \mathcal{R}_N(B) + \epsilon\right] \leq 2Ce^{-N\epsilon^2/2} \tag{48}$$

We can combine this with Eq.(36) to conclude

$$\begin{aligned}
&\Pr\left[\sup_b \|\hat{\mathbb{E}}[Ub(V)] - \mathbb{E}[Ub(V)]\|_2 \geq \sqrt{C}\mathcal{R}_N(B) + \sqrt{C}\epsilon\right] \\
&\leq \Pr\left[\max_c \sup_b \hat{\mathbb{E}}[U^c b(V)] - \mathbb{E}[U^c b(V)]\|_2 \geq \mathcal{R}_N(B) + \epsilon\right] \leq 2Ce^{-N\epsilon^2/2}
\end{aligned}$$

□

Proof of Lemma 4. For B_a^K we use the VC dimension approach. Because $\forall b \in B_a^K$ the set $\{z \in \Delta^C, b(z) = 1\}$ is the intersection of K many C-dimensional half plances, its VC dimension $\mathrm{VC}(B_a^K) \leq (C+1)2K\log_2(3K)$ (Mohri et al., 2018) (Q3.23). By Sauer's Lemma we have

$$\mathcal{R}_N(B_a^K) \leq \sqrt{\frac{2\mathrm{VC}(B_a^K)\log(eN/\mathrm{VC}(B_a^K))}{N}} = O\left(\sqrt{\frac{2CK\log K\log N}{N}}\right)$$

□

E Discussion

Limitations and Social Impact Our results should not be interpreted as guarantees about the quality of individual predictions. For example, the medical provider cannot guarantee to each patient that their expected loss is low. Instead the guarantee should be interpreted as from the machine learning provider to the medical provider (who treats a group of patients). Misuse of our results can lead to unjustified claims about the trust-worthiness of a prediction.

In this paper we only consider loss functions that do not directly depend on the input feature x. Our results can be further extended to include loss functions that depend on the input feature based on the multi-calibration framework. However, when the input feature is complex and high dimensional (e.g. medical images), strong results (such as the feasibility of achieving $\mathcal{L}^K$-decision calibration) becomes much more difficult, and we likely will have to make parametric assumptions on how the loss can depend on the input feature x.