

# A Unified View of Label Shift Estimation

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## Abstract

Label shift describes the setting where although the label distribution might change between the source and target domains, the class-conditional probabilities (of data given a label) do not. There are two dominant approaches for estimating the label marginal. BBSE, a moment-matching approach based on confusion matrices, is provably consistent and provides interpretable error bounds. However, a maximum likelihood estimation approach, which we call MLLS, dominates empirically. In this paper, we present a unified view of the two methods and the first theoretical characterization of the likelihood-based estimator. Our contributions include (i) conditions for consistency of MLLS, which include calibration of the classifier and a confusion matrix invertibility condition that BBSE also requires; (ii) a unified view of the methods, casting the confusion matrix as roughly equivalent to MLLS for a particular choice of calibration method; and (iii) a decomposition of MLLS’s finite-sample error into terms reflecting the impacts of miscalibration and estimation error. Our analysis attributes BBSE’s statistical inefficiency to a loss of information due to coarse calibration. We support our findings with experiments on both synthetic data and the MNIST and CIFAR10 image recognition datasets.

## 1 Introduction

Despite their wide deployment, supervised algorithms are typically developed and evaluated assuming independent and identically distributed (i.i.d) data. However, the real world seldom abides, presenting domain adaptation problems, where the *source distribution*  $P_s$ , from which we sample labeled training examples, differs from the *target distribution*  $P_t$ , from which we only observe unlabeled data. Absent assumptions on the nature of shift, the problem is fundamentally underspecified. Multiple assumptions may be compatible with the same observations while implying different courses of action. Fortunately, some assumptions can render shift detection, estimation, and on-the-fly updates to our classifiers possible.

This paper focuses on *label shift* [Storkey, 2009, Saerens et al., 2002, Lipton et al., 2018], which aligns with a hypothetical *anticausal* setting in which the labels  $y$  cause the features  $x$  [Schölkopf et al., 2012]. Label shift arises in diagnostic problems, because diseases cause symptoms. In this interpretation, an intervention on  $p(y)$  induces the shift, but the process generating  $x$  given  $y$  is fixed ( $p_s(x|y) = p_t(x|y)$ ). Note that in general, under label shift, the optimal predictor (based on  $p(y|x)$ ) changes, e.g., the probability that a patient suffers from a disease given their symptoms can increase under an epidemic. Contrast label shift with the better-known *covariate shift* assumption, which flows from the  $x$  causes  $y$  model, yielding the reverse implication that  $p_s(y|x) = p_t(y|x)$ .

Under label shift, our first task is to estimate the ratios  $w(y) = p_t(y)/p_s(y)$  for all labels  $y$ . Two approaches leverage off-the-shelf classifiers to estimate  $w$ :

1. *Black Box Shift Estimation* (BBSE) [Lipton et al., 2018] and a variant called *Regularized Learning under*

*Label Shift* (RLLS) [Azizzadenesheli et al., 2019]: moment-matching based estimators that leverage (possibly biased, uncalibrated, or inaccurate) predictions to estimate the shift; and

2. Maximum Likelihood Label Shift (MLLS) [Saerens et al., 2002]: an Expectation Maximization (EM) algorithm that estimates  $p_t(y)$  but assumes access to a classifier that outputs the true source distribution conditional probabilities  $p_s(y|x)$ .

Given a predictor  $\hat{f}$  with an invertible confusion matrix, BBSE and RLLS are both provably consistent and offer finite-sample guarantees [Lipton et al., 2018, Azizzadenesheli et al., 2019]. However, absent rigorous theoretical guarantees, MLLS, in combination with Bias-Corrected Temperature Scaling (BCTS), has been shown to outperform them empirically [Alexandari et al., 2019].

In this paper, we provide a theoretical analysis of MLLS, establishing conditions for consistency and bounding its finite-sample error. To start, we observe that given the true label conditional  $p_s(y|x)$ , MLLS is simply a concave Maximum Likelihood Estimation (MLE) problem (not requiring EM) and standard theoretical results apply. However, because we never know  $p_s(y|x)$  exactly, MLLS is always applied with an estimated model  $\hat{f}$  and thus the procedure consists of MLE under model misspecification.

First, we prove that (i) *canonical calibration* and (ii) an invertible confusion matrix (as required by BBSE) are *sufficient conditions* to ensure MLLS’ consistency. Moreover, using binary classification as an example, we prove that calibration can sometimes be *necessary* for consistency (see Example 1 in Section 3.3). Second, we observe that the confusion matrix can be a blunt instrument for calibrating a classifier. Applying MLLS with this technique, BBSE and MLLS are distinguished only by the objective function that they optimize. Through extensive experiments, we show that the two approaches perform similarly, concluding that MLLS’ superior performance (when applied with more granular calibration techniques) is not due to its objective but rather to the information lost by the confusion matrix calibration. Third, we theoretically analyze the finite-sample error of the MLLS estimator by decomposing the error into terms reflecting the miscalibration error and finite-sample error. Depending on the calibration method, the miscalibration error can further be divided into two terms: finite sample error due to re-calibration on a validation set and the minimum achievable calibration error with that technique.

We validate our results on synthetic data and the MNIST and CIFAR-10 image recognition datasets. Empirical results show that MLLS can have  $2\text{--}10\times$  lower Mean Squared estimation Error (MSE) depending on the magnitude of the shift. We experimentally characterize the variation of the MSE as a function of the granularity of the calibration.

In summary, our paper makes the following key contributions:

1. Establishes sufficient conditions for MLLS’ consistency.
2. Unifies label shift estimation methods under a common framework, with BBSE corresponding to a particular choice of calibration method.
3. Derives finite-sample error bounds for MLLS.
4. Supports our theoretical arguments with extensive experiments on synthetic and image recognition datasets.

## 2 Problem Setup and Prior Work

Let  $\mathcal{X}$  be the input space and  $\mathcal{Y} = \{1, 2, \dots, k\}$  the output space. Let  $P_s, P_t : \mathcal{X} \times \mathcal{Y} \rightarrow [0, 1]$  be the source and the target distributions. By  $p_s$  and  $p_t$ , we denote the corresponding probability density (or mass) functions. We use  $\mathbb{E}_s$  and  $\mathbb{E}_t$  to denote expectations over the source and target distributions, respectively. In unsupervised domain adaptation problems, we possess labeled source data  $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$  and unlabeled target data  $\{x_{n+1}, x_{n+2}, \dots, x_{n+m}\}$ . We also assume access to a black-box predictor function  $\hat{f} : \mathcal{X} \mapsto \Delta^{k-1}$ , e.g., a model trained to approximate the true probability function  $f^*$ , where  $f^*(x) :=$

$p_s(\cdot|x)$ . Here and in the rest of the paper, we use  $\Delta^{k-1}$  to denote the standard  $k$ -dimensional probability simplex. For a vector  $v$ , we use  $v_y$  to access the element at index  $y$ .

Absent assumptions relating the source and target distributions, domain adaptation is underspecified [Ben-David et al., 2010]. This paper works under the *label shift* assumption, i.e.,  $p_s(x|y) = p_t(x|y)$ , focusing on multiclass classification problems. Moreover, we assume non-zero support for all labels in the source distribution, i.e., for all  $y \in \mathcal{Y}$   $p_s(y) \geq c > 0$ . Under label shift, three common goals are (i) detection—determining whether distribution shift has occurred; (ii) quantification—estimating the target label distribution; and (iii) correction—producing a predictor that minimizes error on the target distribution [Lipton et al., 2018].

This paper focuses on goal (ii), estimating important weights  $w(y) = p_t(y)/p_s(y)$  for all  $y \in \mathcal{Y}$ . Given  $w$ , we can update our classifiers on the fly, either by retraining with importance-weighted ERM framework [Shimodaira, 2000, Gretton et al., 2009, Lipton et al., 2018, Azizzadenesheli et al., 2019] or by applying an analytic correction using Bayes rule to predicted probabilities (this requires a calibrated classifier to interpret prediction scores as probabilities) [Alexandari et al., 2019, Saerens et al., 2002]. We note that recent empirical results due to Byrd and Lipton [2019] suggest that retraining with importance weights may not be an effective strategy for deep neural networks.

## 2.1 Prior Work on Label Shift Estimation

Two families of solutions have been explored: BBSE [Lipton et al., 2018], a moment matching method, uses the predictor  $\hat{f}$  to compute a confusion matrix  $C_{\hat{f}} := p_s(\hat{y}, y) \in \mathbb{R}^{k \times k}$  on the source data. Depending on how  $\hat{y}$  is defined, there are two types of confusion matrix for a predictor  $\hat{f}$ : (i) the *hard confusion matrix*  $\hat{y} = \arg \max \hat{f}(x)$ ; and (ii) the *soft confusion matrix*, where  $\hat{y}$  is defined as a random prediction that follows the discrete distribution  $\hat{f}(x)$  over  $\mathcal{Y}$ . Both soft and hard confusion matrix can be estimated from labeled source data samples. The estimate  $\hat{w}$  is computed as  $\hat{w} := \hat{C}_{\hat{f}}^{-1} \hat{\mu}$ , where  $\hat{C}_{\hat{f}}$  is the estimate of confusion matrix and  $\hat{\mu}$  is an estimate of  $p_t(\hat{y})$ , computed by applying the predictor  $\hat{f}$  to the target data. In a related vein, RLLS [Azizzadenesheli et al., 2019] incorporates an additional regularization term of the form  $\|w - 1\|$  and solves a constrained optimization problem to estimate the shift ratios  $w$ .

MLLS estimates weights as if performing maximum likelihood estimation, but substitutes the predictor outputs for the true probabilities  $p_s(y|x)$ . Saerens et al. [2002], who introduce this procedure, describe it as an application of EM. However, as observed by Alexandari et al. [2019] (see also Proposition 1), the likelihood objective is concave, and thus a variety of alternative iterative optimization algorithms may be applied to recover the MLLS estimate. Alexandari et al. [2019] also showed that MLLS underperforms BBSE when applied naively, a phenomenon that we shed more light on in this paper. Finally, we note the work of Zhang et al. [2013] which proposed a Maximum Mean Discrepancy (MMD) approach to estimate  $w$ .

## 2.2 Calibration

In contrast to the setting of binary classification, there are multiple possible definitions of calibration in the multiclass setting. Guo et al. [2017] study the calibration of the arg-max prediction, while Kumar et al. [2019] study a notion of per-label calibration. We use canonical calibration [Vaicnavicius et al., 2019] and the expected canonical calibration error, which are defined as follows:

**Definition 1** (Canonical calibration). *A prediction model  $f : \mathcal{X} \mapsto \Delta^{k-1}$  is canonically calibrated if for all  $x \in \mathcal{X}$  and  $j \in \mathcal{Y}$ ,*

$$\mathbb{P}(y = j | f(x)) = f_j(x). \quad (1)$$

**Definition 2** (Expected canonical calibration error). *For a predictor  $f$ , the expected canonical calibration error is*

$$\mathcal{E}(f) = \left( \mathbb{E} \|f - f_c\|^2 \right)^{\frac{1}{2}}, \quad (2)$$

where  $f_c = \mathbb{P}(y = \cdot | f(x))$ .

Absent post-hoc adjustments, neural network predictions tend to be uncalibrated Guo et al. [2017]. Calibration methods typically work either by calibrating the model during training or by calibrating a trained classifier on held-out data, post-hoc. We focus on the latter category of methods. Let the model class used for *post-hoc calibration* be represented by  $\mathcal{G}$ . Given a validation dataset  $\{(x_{v1}, y_{v1}), \dots, (x_{vn}, y_{vn})\}$  sampled from the source distribution  $P_s$  we compute,  $\{(\hat{f}(x_{v1}), y_{v1}), (\hat{f}(x_{v2}), y_{v2}), \dots, (\hat{f}(x_{vn}), y_{vn})\}$ , applying our classifier  $\hat{f}$  to the data. Using this we estimate a function,

$$\hat{g} = \arg \min_{g \in \mathcal{G}} \sum_{i=1}^n \ell(g \circ \hat{f}(x_{vi}), y_{vi}), \quad (3)$$

where the loss function  $\ell$  can be the negative log-likelihood or squared error. Subsequently, we can apply the calibrated predictor  $\hat{g} \circ \hat{f}$ . We refer the interested reader to Kumar et al. [2019] and Guo et al. [2017] for detailed studies on calibration.

Our experiments follow Alexandari et al. [2019], who leverage BCTS<sup>1</sup> to calibrate their models. BCTS extends temperature scaling [Guo et al., 2017] by incorporating per-class bias terms. Formally, a function  $g : \Delta^{k-1} \mapsto \Delta^{k-1}$  in the BCTS class  $\mathcal{G}$ , is given by

$$g_j(x) = \frac{\exp[\log(x_j)/T + b_j]}{\sum_i \exp[\log(x_i)/T + b_i]} \quad \forall j \in \mathcal{Y}$$

where  $\{T, b_1, \dots, b_{|\mathcal{Y}|}\}$  are the  $|\mathcal{Y}| + 1$  parameters to be learned.

### 3 A Unified View of Label Shift Estimation

Given these preliminaries, we can now provide a unified view of label shift estimation and demonstrate how BBSE and MLLS are instantiated under this framework. For now, we assume knowledge of the true  $p_s(x, y)$  and  $p_t(x)$ , deferring a treatment of finite-sample issues to Section 4. For convenience, throughout Sections 3 and 4, we use the term *calibration* exclusively to refer to canonical calibration (Definition 1). We relegate all technical proofs to Appendix A.

#### 3.1 A Unified Distribution Matching View

To start, we introduce a *generalized* distribution matching approach for estimating  $w$ . Under label shift, for any (possibly randomized) mapping from  $\mathcal{X}$  to  $\mathcal{Z}$ , we have that,  $p_s(z|y) = p_t(z|y)$  since,

$$p_s(z|y) = p_t(z|y) = \int_{\mathcal{X}} p(z|x)p(x|y)dx.$$

<sup>1</sup>Motivated by the strong empirical results in Alexandari et al. [2019], we use BCTS in our experiments as a surrogate for canonical calibration.

Throughout the paper, we use the notation  $p(z|y)$  to represent either  $p_s(z|y)$  or  $p_t(z|y)$  (which are identical). We now define a family of distributions over  $\mathcal{Z}$  parameterized by  $w \in \mathcal{W}$  as

$$p_w(z) = \sum_{y=1}^k p(z|y)p_s(y)w_y = \sum_{y=1}^k p_s(z, y)w_y, \quad (4)$$

where  $\mathcal{W} = \left\{ w \mid \forall y, w_y \geq 0 \text{ and } \sum_{y=1}^k w_y p_s(y) = 1 \right\}$ .

When  $w = w^*$ , we have that  $p_w(z) = p_t(z)$ . For fixed  $p(z|x)$ ,  $p_t(z)$  and  $p_s(z, y)$  are known because  $p_t(x)$  and  $p_s(x, y)$  are known. So one potential strategy to estimate  $w^*$  is to find a weight vector  $w$  such that

$$\sum_{y=1}^k p_s(z, y)w_y = p_t(z) \quad \forall z \in \mathcal{Z}. \quad (5)$$

At least one such weight vector  $w$  must exist as  $w^*$  satisfies (5). We now characterize conditions under which the weight vector  $w$  satisfying (5) is unique:

**Lemma 1** (Identifiability). *If the set of distributions  $\{p(z|y) : y = 1, \dots, k\}$  are linearly independent, then for any  $w$  that satisfies (5), we must have  $w = w^*$ . This condition is also necessary in general: if the linear independence does not hold then there exists a problem instance where we have  $w, w^* \in \mathcal{W}$  satisfying (5) while  $w \neq w^*$ .*

Lemma 1 follows from the fact that (5) is a linear system with at least one solution  $w^*$ . This solution is unique when  $p_s(z, y)$  is of rank  $k$ . Assuming that  $p_s(y) > 0$  for all  $y$  (as we have throughout this paper), this is equivalent to the linear independence condition. The linear independence condition in Lemma 1, in general, is sufficient for identifiability for discrete  $\mathcal{Z}$ . However, for continuous  $\mathcal{Z}$ , the linear dependence condition has the undesirable property of being sensitive to changes on sets of measure zero. By changing a collection of linearly dependent distributions on a set of measure zero, we can make them linearly independent. As a consequence, we impose a *stronger* notion of identifiability i.e., the set of distributions  $\{p(z|y) : y = 1, \dots, k\}$  are such that there does not exist  $v \neq 0$  for which

$$\int_{\mathcal{Z}} \left| \sum_y p(z|y)v_y \right| dz = 0. \quad (6)$$

We refer to (6) as *strict linear independence* of the set of distributions  $\{p(z|y) : y = 1, \dots, k\}$ . In generalized distribution matching, one can set  $p(z|x)$  to be the Dirac delta function at  $\delta_x$ <sup>2</sup> such that  $\mathcal{Z}$  is the same space as  $\mathcal{X}$ , which leads to solving (5) with  $z$  replaced by  $x$ . In practice where  $\mathcal{X}$  is high-dimensional and/or continuous, approximating the solution to (5) from finite samples can be hard when choosing  $z = x$ . Our motivation for generalizing distribution matching from  $\mathcal{X}$  to  $\mathcal{Z}$  is that the solution to (5) can be better approximated using finite samples when  $\mathcal{Z}$  is chosen carefully. Under this framework, the design of a label shift estimation algorithm can be decomposed into two parts: (i) the choice of  $p(z|x)$  and (ii) how to approximate the solution to (5). Later on, we consider how these design choices may affect label shift estimation procedures in practice.

### 3.2 The Confusion Matrix Approach

If  $\mathcal{Z}$  is a discrete space, one can first estimate  $p_s(z, y) \in \mathbb{R}^{|\mathcal{Z}| \times k}$  and  $p_t(z) \in \mathbb{R}$ , and then subsequently attempt to solve (5). Confusion matrix approaches use  $\mathcal{Z} = \mathcal{Y}$ , and construct  $p(z|x)$  using a black box predictor  $\hat{f}$ . There are two common choices to construct the confusion matrix:

<sup>2</sup>For simplicity we will use  $z = x$  to denote that  $p(z|x) = \delta_x$ .

1. The soft confusion matrix approach: We set  $p(z|x) := \hat{f}(x) \in \Delta^{k-1}$ . We then define a random variable  $\hat{y} \sim \hat{f}(x)$  for each  $x$ . Then we construct  $p_s(z, y) = p_s(\hat{y}, y)$  and  $p_t(z) = p_t(\hat{y})$ .
2. The hard confusion matrix approach: Here we set  $p(z|x) = \delta_{\arg \max \hat{f}(x)}$ . We then define a random variable  $\hat{y} = \arg \max \hat{f}(x)$  for each  $x$ . Then again we have  $p_s(z, y) = p_s(\hat{y}, y)$  and  $p_t(z) = p_t(\hat{y})$ .

Since  $p_s(z, y)$  is a square matrix, the identifiability condition becomes the invertibility of the confusion matrix. Given an estimated confusion matrix, one can find  $w$  by inverting the confusion matrix (BBSE) or minimizing some distance between the vectors on the two sides of (5).

### 3.3 Maximum Likelihood Label Shift Estimation

When  $\mathcal{Z}$  is a continuous space, the set of equations in (5) indexed by  $\mathcal{Z}$  is intractable. In this case, one possibility is to find a weight vector  $\tilde{w}$  by minimizing the KL-divergence  $\text{KL}(p_t(z), p_w(z)) = \mathbb{E}_t [\log p_t(z)/p_w(z)]$ , for  $p_w$  defined in (4). This is equivalent to maximizing the population log-likelihood:

$$\tilde{w} := \arg \max_{w \in \mathcal{W}} \mathbb{E}_t [\log p_w(z)] . \quad (7)$$

One can further show that

$$\begin{aligned} \mathbb{E}_t [\log p_w(z)] &= \mathbb{E}_t \left[ \log \sum_{y=1}^k p_s(z, y) w_y \right] \\ &= \mathbb{E}_t \left[ \log \sum_{y=1}^k p_s(y|z) p_s(z) w_y \right] \\ &= \mathbb{E}_t \left[ \log \sum_{y=1}^k p_s(y|z) w_y \right] + \mathbb{E}_t [p_s(z)] . \end{aligned}$$

Therefore we can equivalently define:

$$\tilde{w} := \arg \max_{w \in \mathcal{W}} \mathbb{E}_t \left[ \log \sum_{y=1}^k p_s(y|z) w_y \right] . \quad (8)$$

The above optimization problem is convex as shown below. Under the assumption of non-zero support of source labels, i.e., the assumption that for all  $y \in \mathcal{Y}$   $p_s(y) = c > 0$ , the likelihood objective is also bounded from above by  $-\log(c)$ .

**Proposition 1** (Alexandari et al. [2019]). *Optimization problem (8) is convex.*

The proof argument follows simply: Our objective is to minimize the negative log of a convex combination of a linear function in parameters. The minimization is over a convex region and thus the problem is convex.

Assuming access to labeled source data and unlabeled target data, one can maximize the empirical counterpart of the objective in (8), using either EM or an alternative iterative optimization scheme. Saerens et al. [2002] derived an EM algorithm to maximize the objective (8) when  $z = x$ , assuming access to  $p_s(y|x)$ . Absent knowledge of the ground truth  $p_s(y|x)$ , we can plug in any approximate predictor  $f$  and optimize the following objective:

$$w_f := \arg \max_{w \in \mathcal{W}} \mathcal{L}(w, f) := \arg \max_{w \in \mathcal{W}} \mathbb{E}_t [\log f(x)^T w] . \quad (9)$$



In practice,  $f$  is usually fit from a finite number of samples from  $p_s(x, y)$  and standard machine learning methods often produce predictors that are biased or uncalibrated. Unlike BBSE and RLLS, which are provably consistent whenever the predictor  $f$  yields an invertible confusion matrix, to our knowledge, no prior works have established sufficient conditions to guarantee MLLS' consistency when  $f$  differs from  $p_s(y|x)$ .

It is intuitive that for some values of  $f \neq p_s(y|x)$ , MLLS will yield inconsistent estimates. Supplying empirical evidence, Alexandari et al. [2019] show that MLLS performs poorly when  $f$  is a vanilla neural network predictor learned from data. However, Alexandari et al. [2019] also show that in combination with a particular post-hoc calibration technique, MLLS achieves low error, significantly outperforming BBSE and RLLS. As the calibration error is not a distance metric between  $f$  and  $p_s(y|x)$  (zero calibration error does not indicate  $f = p_s(y|x)$ ), a calibrated predictor  $f$  may still be substantially different from  $p_s(y|x)$ . Some natural questions then arise:

1. *Why does calibration improve MLLS so dramatically?*
2. *Is calibration necessary or sufficient to ensure the consistency of MLLS?*
3. *What accounts for the comparative efficiency of MLLS with BCTS calibration over BBSE?*

To address the first two questions, we make the following observations. Suppose we define  $z$  (for each  $x$ ) with distribution,  $p(z|x) := \delta_{f(x)}$ , for some calibrated predictor  $f$ . Then, we observe that as a consequence of the calibration of  $f$ ,  $p_s(y|z) = f(x)$ .

In other words, the MLLS objective (9) can in general be different from that in (8). However, for a particular choice of generalized distribution matching, namely when  $p(z|x) := \delta_{f(x)}$ , the two objectives are identical. The following Lemma formally states this observation:

**Lemma 2.** *If  $f$  is calibrated, then the two objectives (8) and (9) are identical when  $\mathcal{Z}$  is chosen as  $\Delta^{k-1}$  and  $p(z|x)$  is defined to be  $\delta_{f(x)}$ .*

Lemma 2 follows from changing the variable of expectation from  $x$  to  $f(x)$  in (9) and applying  $f(x) = p_s(y|f(x))$  by the definition of calibration. It shows that MLLS with a calibrated predictor on the input space  $\mathcal{X}$  is in fact equivalent to performing distribution matching in the space  $\mathcal{Z}$ . Building on this observation, we are now ready to state our main population-level consistency theorem for MLLS:

**Theorem 1** (Population consistency of MLLS). *If a predictor  $f : \mathcal{X} \mapsto \Delta^{k-1}$  is calibrated and the distributions  $\{p(f(x)|y) : y = 1, \dots, k\}$  are strictly linearly independent, then  $w^*$  is the unique maximizer of the MLLS objective (9).*

The proof of Theorem 1 is a direct combination of Lemma 1, Lemma 2, and an elementary property of the KL-divergence. The population-level consistency of MLLS relies on the linear independence of the collection of distributions  $\{p(f(x)|y) : y = 1, \dots, k\}$ . The following result develops several alternative equivalent characterizations of this linear independence condition.

**Proposition 2.** *For a calibrated predictor  $f$ , the following statements are equivalent:*

- (1)  *$\{p(f(x)|y) : y = 1, \dots, k\}$  are strictly linearly independent.*
- (2)  *$\mathbb{E}_s [f(x)f(x)^T]$  is invertible.*
- (3) *The soft confusion matrix of  $f$  is invertible.*

We now turn our attention to establishing consistency of the sample-based estimator. Let  $x_1, x_2, \dots, x_m \stackrel{iid}{\sim} p_t(x)$ . The finite sample objective for MLLS can be written as

$$\hat{w}_f := \arg \max_{w \in \mathcal{W}} \frac{1}{m} \sum_{i=1}^m \log f(x_i)^T w := \arg \max_{w \in \mathcal{W}} \mathcal{L}_m(w, f). \quad (10)$$

**Theorem 2** (Consistency of MLLS). *If  $f$  satisfies the conditions in Theorem 1, then  $\hat{w}_f$  in (10) converges to  $w^*$  almost surely.*

Having provided sufficient conditions, we consider a binary classification example to provide intuition for why we need calibration for consistency. In this example, we relate the estimation error to the miscalibration error, showing that calibration is not only sufficient but also necessary to achieve zero estimation error for a certain class of predictors.

**Example 1.** Consider a mixture of two Gaussians with  $p_s(x|y=0) := \mathcal{N}(\mu, 1)$  and  $p_s(x|y=1) := \mathcal{N}(-\mu, 1)$ . We suppose that the source mixing coefficients are both  $\frac{1}{2}$ , while the target mixing coefficients are  $\alpha(\neq \frac{1}{2}), 1 - \alpha$ . Assume a class of probabilistic threshold classifiers:  $f(x) = [1 - c, c]$  for  $x \geq 0$ , otherwise  $f(x) = [c, 1 - c]$  with  $c \in [0, 1]$ . Then the population error of MLLS is given by

$$4 \left| \frac{(1 - 2\alpha)(p_s(x \geq 0|y=0) - c)}{1 - 2c} \right|,$$

which is zero only if  $c = p_s(x \geq 0|y=0)$  for a non-degenerate classifier.

The expression for estimation error arising from our example yields two key insights: (i) an uncalibrated thresholded classifier has an estimation error proportional to the true shift in label distribution i.e.  $1 - 2\alpha$ ; (ii) the error is also proportional to the canonical calibration error which is  $p_s(x \geq 0|y=0) - c$ . We formally derive the expression for estimation error in Appendix A. While earlier in this section, we concluded that calibration is sufficient for consistency, the above example provides some intuition for why calibration might also be necessary.

### 3.4 MLLS with Confusion Matrix

So far, we have shown that MLLS with any calibrated predictor can be viewed as distribution matching in a latent space. Now we come to the question of whether we can construct a predictor  $f$  to perform MLLS given any  $p(z|x)$ , e.g., those induced by confusion matrix approaches. As we already have the maximum log-likelihood objective given any  $p(z|x)$  in (8), it remains to construct a predictor  $f$  such that one can rewrite (8) as (9). This is straightforward when  $p(z|x)$  is deterministic, i.e.,  $p(z|x) = \delta_{g(x)}$  for some function  $g$ : setting  $f(x) = p_s(y|g(x))$  makes the two objectives to be the same. Recall that for the hard confusion matrix, the induced latent space is  $p(z|x) = \delta_{\arg \max \hat{f}(x)}$ . So the corresponding predictor in MLLS is  $f(x) = p_s(y|\hat{y}_x)$ , where  $\hat{y}_x = \arg \max \hat{f}(x)$ . Then we obtain the MLLS objective for the hard confusion matrix:

$$\max_{w \in \mathcal{W}} \mathbb{E}_t \left[ \log \sum_{y=1}^k p_s(y|\hat{y}_x) w_y \right]. \quad (11)$$

The confusion matrix  $C_{\hat{f}}$  and predictor  $\hat{f}$  directly give us  $p_s(y|\hat{y}_x)$ : Given an input  $x$ , one can first get  $\hat{y}_x$  from  $\hat{f}$ , then normalize the  $\hat{y}_x$ -th row of  $C_{\hat{f}}$  as  $p_s(y|\hat{y}_x)$ . The predictor constructed in this way is calibrated and thus suitable for application with MLLS.

**Proposition 3** (Proposition 1 from Vaicenavicius et al. [2019]). *For any function  $g$ ,  $f(x) = p_s(y|g(x))$  is a calibrated predictor.*

When  $p_s(z|x)$  is stochastic, we need to extend (9) to allow  $f$  to be a random predictor:  $f(x) = p_s(y|z)$  for  $z \sim p(z|x)$ <sup>3</sup>. To incorporate the randomness of  $f$ , one only needs to change the expectation in (9) to be

<sup>3</sup>Here, by a random predictor we mean that the predictor outputs a random vector from  $\Delta^{k-1}$ , not  $\mathcal{Y}$ .



over both  $x$  and  $f(x)$ , then (9) becomes a rewrite of (8). Again, the random predictor is calibrated and we can have an MLLS objective for the soft confusion matrix approach.

Proposition 3 indicates that constructing the confusion matrix is a calibration procedure: for any black box predictor  $\hat{f}$ , one can obtain a calibrated predictor  $f$  from its confusion matrix  $C_{\hat{f}}$ . We can now summarize the relationship between BBSE and MLLS:

A label shift estimator involves two design choices: (i) designing the latent space  $p(z|x)$  (which is equivalent to designing a calibrated predictor); and (ii) performing distribution matching in the new space  $\mathcal{Z}$ . In BBSE, we design a calibrated predictor via the confusion matrix and then perform distribution matching by directly solving linear equations. In general, MLLS does not specify how to obtain a calibrated predictor, but specifies KL minimization as the distribution matching procedure. One can apply the confusion matrix approach to obtain a calibrated predictor and then plug it into MLLS, which is the BBSE analog under MLLS, and is a special case of MLLS.

## 4 Theoretical Analysis of MLLS

We now analyze the performance of MLLS estimators. Even when  $w^*$  is the unique optimizer of (9) for some calibrated predictor  $f$ , assuming convex optimization can be done perfectly, there are still two sources of error preventing us from exactly computing  $w^*$  in practice. First, we are optimizing a sample-based approximation (10) to the objective in expectation (9). We call this source of error *finite-sample error*. Second, the predictor  $f$  we use may not be perfectly calibrated. Perfect calibration might require full access to the source data distribution  $p_s(x, y)$ , while we only have access to a sample from this distribution. We call this source of error *miscalibration error*. In this section, we will first analyze how these two sources of errors affect the estimate of  $w^*$  separately and then give a general error bound that incorporates both. All proofs are relegated to Appendix B.

Before presenting our analysis, we introduce some notation and regularity assumptions. For any predictor  $f : \mathcal{X} \mapsto \Delta^{k-1}$ , we define  $w_f$  and  $\hat{w}_f$  as in (9) and (10). If  $f$  satisfies the conditions in Theorem 1 (calibration and linear independence) then we have that  $w_f = w^*$ . Our goal is to bound  $\|\hat{w}_f - w^*\|$  for a given (possibly miscalibrated) predictor  $f$ . We now introduce a regularity condition for a predictor  $f$ :

**Condition 1** (Regularity condition for a predictor  $f$ ). *For any  $x$  within the support of  $p_t(x)$ , i.e.  $p_t(x) > 0$ , we have both  $f(x)^T w_f \geq \tau$ ,  $f(x)^T w^* \geq \tau$  for some universal constant  $\tau > 0$ .*

Condition 1 is mild if  $f$  is calibrated since in this case  $w_f = w^*$  is the maximizer of  $\mathbb{E}_t [\log f(x)^T w]$ , and the condition is satisfied if the expectation is finite. Since  $f(x)^T w^*$  and  $f(x)^T w_f$  are upper-bounded (they are the inner products of two vectors which sum to 1), they also must be lower-bounded away from 0 with arbitrarily high probability without any assumptions. For miscalibrated  $f$ , a similar justification holds for assumption that  $f(x)^T w_f$  is lower bounded. Turning our attention to the assumption that  $f(x)^T w^*$  is lower bounded, we note that it is sufficient if  $f$  is close (pointwise) to some calibrated predictor. This in turn is a reasonable assumption on the actual predictor we use for MLLS in practice as it is post-hoc calibrated on source data samples.

Define  $\sigma_{f,w}$  to be the minimum eigenvalue of the Hessian  $-\nabla_w^2 \mathcal{L}(w, f)$ . To state our results compactly we use standard stochastic order notation (see, for instance, [van der Vaart and Wellner, 1996]). We first bound the estimation error introduced by only having finite samples from the target distribution:

**Lemma 3.** *For any predictor  $f$  that satisfies Condition 1, we have*

$$\|w_f - \hat{w}_f\| \leq \sigma_{f,w_f}^{-1} \cdot \mathcal{O}_p \left( m^{-1/2} \right). \quad (12)$$

We now bound the estimation error introduced by having a miscalibrated  $f$ :

**Lemma 4.** *For any predictor  $f$  and any calibrated predictor  $f_c$  that satisfies Condition 1, we have*

$$\|w_f - w^*\| \leq \sigma_{f,w^*}^{-1} \cdot C \cdot \mathbb{E}_t [\|f - f_c\|], \quad (13)$$

for some constant  $C$ .

If we set  $f_c(x) = p_s(y|f(x))$ , which is a calibrated predictor according to Proposition 3, we can further bound the error in terms of the calibration error of  $f$ <sup>4</sup>:

$$\|w_f - w^*\| \leq \sigma_{f,w^*}^{-1} \cdot C \cdot \mathcal{E}(f). \quad (14)$$

We formally prove these lemmas in Appendix B but give a proof sketch here. Lemmas 3 and 4 bound the difference between the optimizers of two different functions. The proof starts with a second-order Taylor expansion of one function around the optimum of the other function. Using this Taylor expansion, we relate the estimation error to the difference between the gradient of two functions evaluated at the same point, e.g.,  $\|\nabla_w \mathcal{L}_m(w_f, f) - \nabla_w \mathcal{L}(w_f, f)\|$  for Lemma 3 and  $\|\nabla_w \mathcal{L}(w^*, f) - \nabla_w \mathcal{L}(w^*, f_c)\|$  for Lemma 4. For Lemma 3, we then use a concentration inequality to bound the difference in gradients, while for Lemma 4, we exploit the Lipschitzness of the gradient to relate the difference in gradients to the difference in function values.

We combine the two sources of error to get a bound on the estimation error  $\|\hat{w}_f - w^*\|$ :

**Theorem 3.** *For any predictor  $f$  that satisfies Condition 1, we have*

$$\|\hat{w}_f - w^*\| \leq \sigma_{f,w_f}^{-1} \mathcal{O}_p(m^{-1/2}) + C \cdot \sigma_{f,w^*}^{-1} \mathcal{E}(f). \quad (15)$$

The estimation error of MLLS can be decomposed into (i) finite-sample error, which decays at a rate of  $m^{-1/2}$ ; and (ii) the calibration error of the predictor that we use. The proof is a direct combination of Lemma 3 and Lemma 4 applied to the same  $f$  with the following error decomposition:

$$\|\hat{w}_f - w^*\| \leq \underbrace{\|w_f - \hat{w}_f\|}_{\text{finite-sample}} + \underbrace{\|w_f - w^*\|}_{\text{miscalibration}}.$$

Theorem 3 also shows that the estimation error depends inversely on the minimum eigenvalue of the Hessian at two different points  $w_f$  and  $w^*$ . One can further unify these two eigenvalues as a single quantity by the following observation:

**Proposition 4.** *For any  $w \in \mathcal{W}$ , we have  $\sigma_{f,w} \geq p_{s,\min} \sigma_f$  where  $\sigma_f$  is the minimum eigenvalue of  $\mathbb{E}_t [f(x)f(x)^T]$  and  $p_{s,\min} = \min_{y \in \mathcal{Y}} p_s(y)$ . Furthermore, if  $f$  satisfies Condition 1, we have*

$$p_{s,\min}^2 \cdot \sigma_f \leq \sigma_{f,w} \leq \tau^{-2} \cdot \sigma_f \quad (16)$$

for  $w \in \{w_f, w^*\}$ .

Proposition 4 shows that we can combine the two eigenvalues in Theorem 3 to a single  $\sigma_f$  and this relaxation is tight up to the factors described in (16).

If we use the *post-hoc calibration* procedure as introduced in Section 2 to calibrate a blackbox predictor  $\hat{f}$ , we can obtain a bound on the calibration error of  $f$ . In more detail, suppose that the class  $\mathcal{G}$  used for calibration satisfies standard regularity conditions (injectivity, Lipschitz-continuity, twice differentiability, non-singular Hessian) described in detail in Theorem 5.23 of Stein [1981]. We have the following lemma:

<sup>4</sup>We present two upper bounds because the second is more interpretable while the first is tighter.

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**Algorithm 1** Maximum Likelihood Label Shift estimation

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**input** : Labeled validation samples from source and unlabeled test samples from target. Trained blackbox model  $\hat{f}$ , model class  $\mathcal{G}$  and loss function  $l$  for calibration.

- 1: On validation data minimize the loss  $l$  over class  $\mathcal{G}$  to obtain  $f = g \circ \hat{f}$ .
- 2: Solve the optimization problem (10) using  $f$  to get  $\hat{w}$ .

**output** : MLLS estimate  $\hat{w}$

---

**Lemma 5.** *Let  $f = g \circ \hat{f}$  be the predictor after post-hoc calibration with squared loss  $l$  and  $g$  belongs to a function class  $\mathcal{G}$  that satisfies the standard regularity conditions, we have*

$$\mathcal{E}(f) \leq \min_{g \in \mathcal{G}} \mathcal{E}(g \circ \hat{f}) + \mathcal{O}_p \left( n^{-1/2} \right). \quad (17)$$

This result is similar to Theorem 4.1 Kumar et al. [2019]. For a model class  $\mathcal{G}$  that is rich enough to contain a function  $g \in \mathcal{G}$  that achieves zero calibration error, i.e.,  $\min_{g \in \mathcal{G}} \mathcal{E}(g \circ \hat{f}) = 0$ , then we obtain an estimation error bound for MLLS of  $\sigma_f^{-1} \cdot \mathcal{O}_p \left( m^{-1/2} + n^{-1/2} \right)$ . This bound is similar to rate of RLLS and BBSE, where instead of  $\sigma_f$  they have minimum eigenvalue of the confusion matrix.

If  $f$  is calibrated, Theorem 3, together with Proposition 4, implies that MLLS is consistent if  $\mathbb{E}_t [f(x)f(x)^T]$  is invertible. Compared to the consistency condition in Theorem 1 that  $\mathbb{E}_s [f(x)f(x)^T]$  is invertible (together with Proposition 2), these two conditions are the same if the likelihood ratio  $p_t(f(x))/p_s(f(x))$  is lower-bounded. This is true if all entries in  $w^*$  are non-zero. Even if  $w^*$  contains non-zero entries, the two conditions are still the same if there exists some  $w_y^* > 0$  such that  $p(f(x)|y)$  covers the full support of  $p_s(f(x))$ . In general however, the invertibility of  $\mathbb{E}_t [f(x)f(x)^T]$  is a stronger requirement than the invertibility of  $\mathbb{E}_s [f(x)f(x)^T]$ . We leave further investigation of this gap for future work.

## 5 Experiments

We experimentally illustrate the performance of MLLS on synthetic data, MNIST [LeCun et al., 1998], and CIFAR10 [Krizhevsky and Hinton, 2009]. Following Lipton et al. [2018], we experiment with *Dirichlet shift* simulations. On each run, we sample a target label distribution  $p_t(y)$  from a Dirichlet with concentration parameter  $\alpha$ . We then generate each target example by first sampling a label  $y \sim p_t(y)$  and then sampling (with replacement) an example conditioned on that label. Note that smaller values of alpha correspond to more severe shift. In our experiments, the source label distribution is uniform.

First, we consider a mixture of two Gaussians (as in Example in Section 3.3) with  $\mu = 1$ . With CIFAR10 and MNIST, we split the full training set into two subsets: train and valid, and use the provided test set as is. Then according to the label distribution, we randomly sample with replacement train, valid, and test set from each of their respective pool to form the source and target set. To learn the black box predictor on real datasets, we use the same architecture as Lipton et al. [2018] for MNIST, and for CIFAR10 we use ResNet-18 [He et al., 2016] as in Azizzadenesheli et al. [2019]<sup>5</sup>. For simulated data, we use the true  $p_s(y|x)$  as our predictor function. For each experiment, we sample 100 datasets for each shift parameter and evaluate the empirical MSE and variance of the estimated weights.

We consider three sets of experiments: (1) MSE vs degree of target shift; (2) MSE vs target sample sizes; and (3) MSE vs calibrated predictors on the source distribution. We refer to MLLS-CM as MLLS with hard confusion matrix calibration as in (11). In our experiments, we compare MLLS estimator with BBSE, RLLS,

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<sup>5</sup>We used open source implementation of ResNet-18 <https://github.com/kuangliu/pytorch-cifar>.

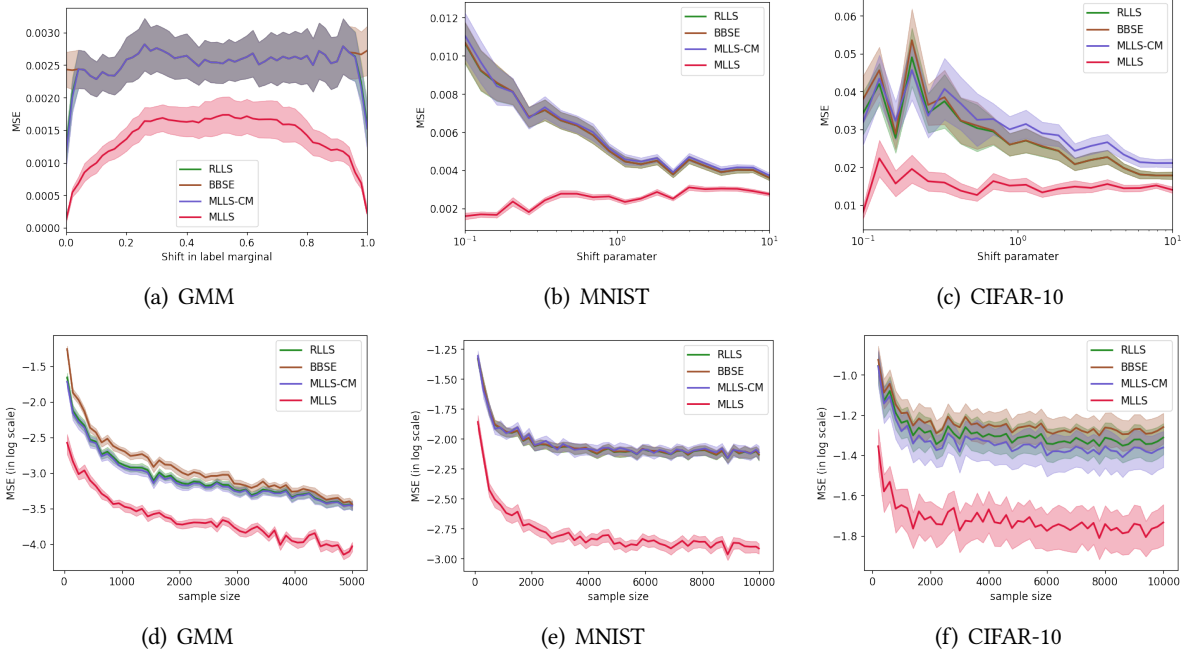


Figure 1: **(top)** MSE vs the degree of shift; For GMM we control the shift in the label marginal for class 1 with a fixed target sample size of 1000 whereas for multiclass problems, MNIST and CIFAR-10, we control the Dirichlet shift parameter with a fixed sample size of 5000. **(bottom)** MSE (in log scale) vs target sample size; For GMM we fix the label marginal for class 1 at 0.01 whereas for multiclass problems, MNIST and CIFAR-10, we fix the Dirichlet parameter to 0.1. In all plots MLLS dominates other methods. All confusion matrix approaches perform similarly, indicating that the advantage of MLLS over BBSE comes from the choice of calibration but not the way of performing distribution matching.

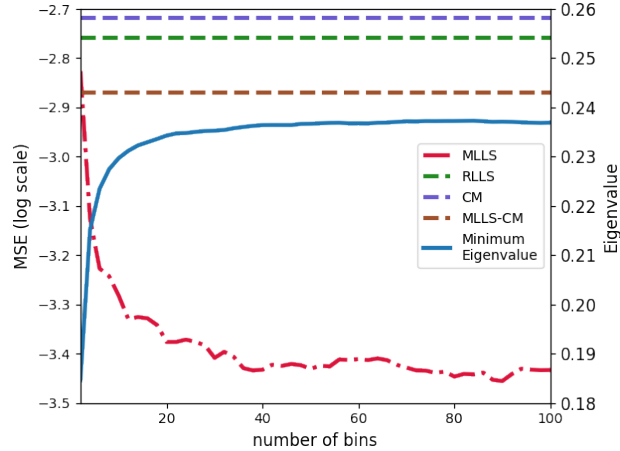


Figure 2: MSE (left-axis) with variation of minimum eigenvalue of the Hessian (right-axis) vs number of bins used for aggregation. With increase in number of bins, MSE decrease and the minimum eigenvalue increases.

and MLLS-CM. For RLLS and BBSE, we use the publicly available code <sup>6</sup>. To post-hoc calibration, we use

<sup>6</sup>BBSE: [https://github.com/zackchase/label\\_shift](https://github.com/zackchase/label_shift), RLLS: <https://github.com/Angela0428/labelshift>

BCTS [Alexandari et al., 2019] on the held-out validation set. Using the same validation set, we calculate the confusion matrix for BBSE, RLLS, and MLLS-CM.

We examine the performance of various estimators across all three datasets for various target dataset sizes and shift magnitudes (Figure 1). Across all shifts, MLLS (with BCTS-calibrated classifiers) *uniformly dominates* BBSE, RLLS, and MLLS-CM in terms of MSE (Figure 1). Observe for severe shifts, MLLS is comparatively dominant. As the available target data increased, all methods improve rapidly, with MLLS outperforming all other methods by a significant margin. Confirming the findings of Alexandari et al. [2019], MLLS’ advantages grow more pronounced under extreme shifts. Notice MLLS-CM is roughly equivalent to BBSE across all settings of dataset, target size, and shift magnitude. This concludes MLLS’ superior performance is not because of differences in loss function used for distribution matching but due to differences in the granularity of the predictions, caused by crude confusion matrix aggregation.

Note that given a predictor  $f_1$ , we can partition our input space and produce another predictor  $f_2$  that, for any data point gives the expected output of  $f_1$  on points belonging to that partition. If  $f_1$  is calibrated, then  $f_2$  will also be calibrated [Vaicenavicius et al., 2019]. On synthetic data, we vary the granularity of calibrated predictors by aggregating  $p_s(y|x)$  over different number of equal sized bins. As the number of bins grows larger, less information is lost by virtue of calibration. Consequently, the minimum eigenvalue of the Hessian increases and MSE for MLLS decreases, verifying our theoretical bounds. Note that these experiments presume access to the true predictor  $p_s(y|x)$  and thus the MSE strictly improves with the number of bins. In practice, with a fixed source dataset size, increasing the number of bins could lead to overfitting, worsening our calibration.

## 6 Conclusion

This paper provides a unified framework relating techniques for label shift estimation. We argue that these methods all employ calibration, either explicitly or implicitly, differing only in the choice of calibration method and their optimization objective. Moreover, we experimentally show that the choice of calibration method (and not the optimization objective for distribution matching) accounts for the noted advantage of MLLS (with BTCS calibration) over BBSE. In future work, we hope to operationalize these insights to provide guidance for how to optimize a calibration scheme to minimize downstream label shift estimation error.

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## A Proofs from Section 3

**Lemma 1** (Identifiability). *If the set of distributions  $\{p(z|y) : y = 1, \dots, k\}$  are linearly independent, then for any  $w$  that satisfies (5), we must have  $w = w^*$ . This condition is also necessary in general: if the linear independence does not hold then there exists a problem instance where we have  $w, w^* \in \mathcal{W}$  satisfying (5) while  $w \neq w^*$ .*

*Proof.* First we prove sufficiency. If there exists  $w \neq w^*$  such that (5) holds, then we have  $\sum_{y=1}^k p_s(z, y)(w_y - w_y^*) = 0$  for all  $z \in \mathcal{Z}$ . As  $w - w^*$  is not the zero vector,  $\{p_s(z, y), y = 1, \dots, k\}$  are linearly dependent. Since  $p_s(z, y) = p_s(y)p(z|y)$  and  $p_s(y) > 0$  for all  $y$  (by assumption), we also have that  $\{p(z|y), y = 1, \dots, k\}$  are linearly dependent. By contradiction, we show that the linear independence is necessary.

To show necessity, assume  $w_y^* = \frac{1}{kp_s(y)}$  for  $y = 1, \dots, k$ . We know that  $w^*$  satisfies (5) by definition. If linear independence does not hold, then there exists a vector  $v \in \mathbb{R}^k$  such that  $v \neq 0$  and  $\sum_{y=1}^k p_s(z, y)v_y = 0$  for all  $z \in \mathcal{Z}$ . Since the  $w^*$  we construct is not on the boundary of  $\mathcal{W}$ , we can scale  $v$  such that  $w^* + \alpha v \in \mathcal{W}$  where  $\alpha \geq 0$  and  $v \neq 0$ . Therefore, setting  $w = w^* + \alpha v$  gives another solution for (5), which concludes the proof.  $\square$

**Lemma 2.** *If  $f$  is calibrated, then the two objectives (8) and (9) are identical when  $\mathcal{Z}$  is chosen as  $\Delta^{k-1}$  and  $p(z|x)$  is defined to be  $\delta_{f(x)}$ .*

*Proof.* The proof follows a sequence of straightforward manipulations. In more detail,

$$\begin{aligned} \mathbb{E}_t [\log f(x)^T w] &= \int p_t(x) \log[f(x)^T w] dx \\ &= \int \int p_t(x) p(z|x) \log[f(x)^T w] dx dz \\ &= \int \int p_t(x) p(z|x) \mathbb{1}\{f(x) = z\} \log[f(x)^T w] dx dz \\ &= \int \int p_t(x) p(z|x) \log[z^T w] dx dz \\ &= \int p_t(z) \log[z^T w] dz \\ &= \int p_t(z) \log \left[ \sum_{y=1}^k p_s(y|z) w \right] dz, \end{aligned}$$

where the final step uses the fact that  $f$  is calibrated.  $\square$

**Theorem 1** (Population consistency of MLLS). *If a predictor  $f : \mathcal{X} \mapsto \Delta^{k-1}$  is calibrated and the distributions  $\{p(f(x)|y) : y = 1, \dots, k\}$  are strictly linearly independent, then  $w^*$  is the unique maximizer of the MLLS objective (9).*

*Proof.* According to Lemma 2 we know that maximizing (9) is the same as maximizing (8) with  $p(z|x) = \delta_{f(x)}$ , thus also the same as minimizing the KL divergence between  $p_t(z)$  and  $p_w(z)$ . Since  $p_t(z) \equiv p_{w^*}(z)$  we know that  $w^*$  is a minimizer of the KL divergence such that the KL divergence is 0. We also have that  $\text{KL}(p_t(z), p_w(z)) = 0$  if and only if  $p_t(z) \equiv p_w(z)$ , so all maximizers of (9) should satisfy (5). According to Lemma 1, if the strict linear independence holds, then  $w^*$  is the unique solution of (5). Thus  $w^*$  is the unique maximizer of (9).  $\square$

**Proposition 2.** For a calibrated predictor  $f$ , the following statements are equivalent:

- (1)  $\{p(f(x)|y) : y = 1, \dots, k\}$  are strictly linearly independent.
- (2)  $\mathbb{E}_s [f(x)f(x)^T]$  is invertible.
- (3) The soft confusion matrix of  $f$  is invertible.

*Proof.* We first show the equivalence of (1) and (2). If  $f$  is calibrated, we have  $p_s(f(x))f_y(x) = p_s(y)p(f(x)|y)$  for any  $x, y$ . Then for any vector  $v \in \mathbb{R}^k$  we have

$$\sum_{y=1}^k v_y p(f(x)|y) = \sum_{y=1}^k \frac{v_y}{p_s(y)} p_s(y) p(f(x)|y) = \sum_{y=1}^k \frac{v_y}{p_s(y)} p_s(f(x)) f_y(x) = p_s(f(x)) \sum_{y=1}^k \frac{v_y}{p_s(y)} f_y(x). \quad (18)$$

On the other hand, we can have

$$\mathbb{E}_s [f(x)f(x)^T] = \int f(x)f(x)^T p_s(f(x)) d(f(x)). \quad (19)$$

If  $\{p(f(x)|y) : y = 1, \dots, k\}$  are linearly dependent, then there exist  $v \neq 0$  such that (18) is zero for any  $x$ . Consequently, there exists a non-zero vector  $u$  with  $u_y = v_y/p_s(y)$  such that  $u^T f(x) = 0$  for any  $x$  satisfying  $p_s(f(x)) > 0$ , which means  $u^T \mathbb{E}_s [f(x)f(x)^T] u = 0$  and thus  $\mathbb{E}_s [f(x)f(x)^T]$  is not invertible. On the other hand, if  $\mathbb{E}_s [f(x)f(x)^T]$  is non-invertible, then there exist some  $u \neq 0$  such that  $u^T \mathbb{E}_s [f(x)f(x)^T] u = 0$ . Further as  $u^T \mathbb{E}_s [f(x)f(x)^T] u = \int u^T f(x)f(x)^T u p_s(x) dx = \int |f(x)^T u| p_s(x) dx$ . As a result, the vector  $v$  with  $v_y = p_s(y)u_y$  satisfies that (18) is zero for any  $x$ , which means  $\{p(f(x)|y) : y = 1, \dots, k\}$  are not strictly linearly independent.

Let  $C$  be the soft confusion matrix of  $f$ , then

$$\begin{aligned} C_{ij} &= p_s(\hat{y} = i, y = j) = \int d(f(x)) f_i(x) p(f(x)|y = j) p_s(y = j) \\ &= \int f_i(x) f_j(x) p_s(f(x)) d(f(x)). \end{aligned}$$

Therefore, we have  $C = \mathbb{E}_s [f(x)f(x)^T]$ , which means (2) and (3) are equivalent.  $\square$

We introduce some notation before proving consistency. Let  $\mathcal{P} = \{\langle f, w \rangle | w \in \mathcal{W}\}$  be the class of densities<sup>7</sup> for a given calibrated predictor  $f$ . Suppose  $\hat{p}_n, p_0 \in \mathcal{P}$  are densities corresponding to MLE estimate and true weights, respectively. We use  $h(p_1, p_2)$  to denote the Hellinger distance and  $\text{TV}(p_1, p_2)$  to denote the total variation distance between two densities  $p_1, p_2$ .  $H_r(\delta, \mathcal{P}, P)$  denotes  $\delta$ -entropy for class  $\mathcal{P}$  with respect to metric  $L_r(P)$ . Similarly,  $H_{r,B}(\delta, \mathcal{P}, P)$  denotes the corresponding bracketing entropy. Moreover,  $P_n$  denotes the empirical random distribution that puts uniform mass on observed samples  $x_1, x_2, \dots, x_n$ . Before proving consistency we need to re-state two results:

**Lemma 6** (Lemma 2.1 van de Geer [2000]). If  $P$  is a probability measure, for all  $1 \leq r < \infty$ , we have

$$H_{r,B}(\delta, \mathcal{G}, P) \leq H_\infty(\delta/2, \mathcal{G}) \quad \text{for all } \delta > 0.$$

<sup>7</sup>Note that we use the term *density* loosely here for convenience. The actual density is  $\langle f(x), w \rangle \cdot p_s(x)$  but we can ignore  $p_s(x)$  because it does not depend on our parameters.

**Lemma 7** (Corollary 2.7.10 [van der Vaart and Wellner \[1996\]](#)). Let  $\mathcal{F}$  be the class of convex functions  $f : C \mapsto [0, 1]$  defined on a compact, convex set  $C \subset \mathbb{R}^d$  such that  $|f(x) - f(y)| \leq L \|x - y\|$  for every  $x, y$ . Then

$$H_\infty(\delta, \mathcal{F}) \leq K \left( \frac{L}{\delta} \right)^{d/2},$$

for a constant  $K$  that depends on the dimension  $d$  and  $C$ .

We can now present our proof of consistency, which is based on Theorem 4.6 from [van de Geer \[2000\]](#):

**Lemma 8** (Theorem 4.6 [van de Geer \[2000\]](#)). Let  $\mathcal{P}$  be convex and define class  $\mathcal{G} = \left\{ \frac{2p}{p+p_0} \mid p \in \mathcal{P} \right\}$ . If

$$\frac{1}{n} H_1(\delta, \mathcal{G}, P_n) \rightarrow_P 0, \quad (20)$$

then  $h(\hat{p}_n, p_0) \rightarrow 0$  almost surely.

**Theorem 2** (Consistency of MLLS). If  $f$  satisfies the conditions in Theorem 1, then  $\hat{w}_f$  in (10) converges to  $w^*$  almost surely.

*Proof.* Assume the maximizer of (10) is  $\hat{w}_f$  and  $p_0 = \langle f, w^* \rangle$ . Define class  $\mathcal{G} = \left\{ \frac{2p}{p+p_0} \mid p \in \mathcal{P} \right\}$ . To prove consistency, we first bound the bracketing entropy for class  $\mathcal{G}$  using Lemma 6 and Lemma 7.

Clearly  $\mathcal{P}$  is linear in parameters and hence, convex. Gradient of function  $g \in \mathcal{G}$  is given by  $\frac{2p_0}{(p+p_0)^2}$  which in turn is bounded by  $\frac{2}{p_0}$ . Under assumptions of Condition 1, the functions in  $\mathcal{G}$  are Lipschitz with constant  $2/\tau$ . We can bound the bracketing entropy  $H_{2,B}(\delta, \mathcal{G}, P)$  using Lemma 7 and Lemma 6 as

$$H_{2,B}(\delta, \mathcal{G}, P) \leq H_\infty(\delta, \mathcal{G}) \leq K_1 \left( \frac{1}{\delta\tau} \right)^{k/2},$$

for some constant  $K_1$  that depends on  $k$ .

On the other hand, for cases where  $p_0$  can be arbitrarily close to zero, i.e., Condition 1 doesn't hold true, we define  $\tau(\delta)$  and  $\mathcal{G}_\tau$  as

$$\begin{aligned} \tau(\delta) &= \sup \left\{ \tau \geq 0 \mid \int_{p_0 \leq \tau} p_0 dx \leq \delta^2 \right\}, \\ \mathcal{G}_\tau &= \left\{ \frac{2p}{p+p_0} \mathbb{1}_{\{p_0 \geq \tau\}} \mid p \in \mathcal{P} \right\}. \end{aligned} \quad (21)$$

Using triangle inequality, for any  $g_1, g_2 \in \mathcal{G}$ , we have

$$\begin{aligned} \int \|g_1 - g_2\|^2 dx &\leq \int \|g_1 - g_2\|^2 \mathbb{1}_{\{p_0 \leq \tau\}} dx + \int \|g_1 - g_2\|^2 \mathbb{1}_{\{p_0 \geq \tau\}} dx \\ &\leq 2 \int \mathbb{1}_{\{p_0 \leq \tau\}} dx + \int \|g_1 - g_2\|^2 \mathbb{1}_{\{p_0 \geq \tau\}} dx. \end{aligned} \quad (22)$$

Assume  $\tau(\delta)$  such that (21) is satisfied. Using (22), we have

$$H_{2,B}(\delta, \mathcal{G}, P) \leq H_{2,B}(\sqrt{3}\delta, \mathcal{G}_{\tau(\delta)}, P).$$

Thus, for the cases where  $p_0$  can be arbitrarily close to zero, instead of bounding  $H_{2,B}(\delta, \mathcal{G}, P)$ , we bound  $H_B(\delta, \mathcal{G}_{\tau(\delta)}, P)$ . For any  $\delta > 0$ , there is a compact subset  $K_\delta \in \mathcal{X}$ , such that  $p_s(X \setminus K_\delta) < \delta$ .

Using arguments similar to above, function  $g \in \mathcal{G}_{\tau(\delta)}$  is Lipschitz with constant  $2/\tau(\delta) > 0$ . Again using Lemma 7 and Lemma 6, we conclude

$$H_{2,B}(2\delta, \mathcal{G}_{\tau(\delta)}, P) \leq H_{\infty}(\delta, \mathcal{G}_{\tau(\delta)}) \leq K_2 \left( \frac{1}{\delta\tau(\delta)} \right)^k,$$

for some constant  $K_2$  that depends on  $k$ . Finally, we use Lemma 8 to conclude  $h(\hat{p}_n, p_0) \rightarrow_{\text{a.s.}} 0$ . Further, as  $\text{TV}(\hat{p}_n, p_0) \leq h(\hat{p}_n, p_0)$ , we have  $h(\hat{p}_n, p_0) \rightarrow_{\text{a.s.}} 0$  implies  $\text{TV}(\hat{p}_n, p_0) \rightarrow_{\text{a.s.}} 0$ . Further

$$\begin{aligned} \|\hat{w}_f - w^*\|^2 &\leq \frac{1}{\lambda_{\min}} \int |f(x)^T(\hat{w}_f - w^*)|^2 p_s(x) dx \\ &\leq \frac{\sup_x \{|f(x)^T(\hat{w}_f - w^*)|\}}{\lambda_{\min}} \underbrace{\int |f(x)^T(\hat{w}_f - w^*)| p_s(x) dx}_{\text{TV}(\hat{p}_n, p_0)}, \end{aligned} \quad (23)$$

where  $\lambda_{\min}$  is the minimum eigenvalue of covariance matrix  $[\int f(x)f(x)^T p_s(x) dx]$ . Note using Proposition 2, we have  $\lambda_{\min} > 0$ . Thus, we conclude  $\|\hat{w}_f - w^*\| \rightarrow_{\text{a.s.}} 0$ .  $\square$

**Example 1.** Consider a mixture of two Gaussians with  $p_s(x|y=0) := \mathcal{N}(\mu, 1)$  and  $p_s(x|y=1) := \mathcal{N}(-\mu, 1)$ . We suppose that the source mixing coefficients are both  $\frac{1}{2}$ , while the target mixing coefficients are  $\alpha(\neq \frac{1}{2}), 1 - \alpha$ . Assume a class of probabilistic threshold classifiers:  $f(x) = [1 - c, c]$  for  $x \geq 0$ , otherwise  $f(x) = [c, 1 - c]$  with  $c \in [0, 1]$ .

Then the population error of MLLS is given by

$$4 \left| \frac{(1 - 2\alpha)(p_s(x \geq 0|y=0) - c)}{1 - 2c} \right|,$$

which is zero only if  $c = p_s(x \geq 0|y=0)$  for a non-degenerate classifier.

*Proof.* The intuition behind the construction is, for such an Example, we can get a closed form solution for the population MLLS and hence allows a careful analysis of the estimation error. The classifier  $f(x)$  predicts class 0 with probability  $c$  and class 1 with probability  $1 - c$  for  $x \geq 0$ , and vice-versa for  $x < 0$ . Using such a classifier, the weight estimator is given by:

$$\begin{aligned} \hat{w} &= \arg \min_w \mathbb{E} [\log \langle f(x), w \rangle] \\ &\stackrel{(i)}{=} \arg \min_{w_0} \left[ \int_{-\infty}^0 \log((1 - c)w_0 + c(2 - w_0)) p_t(x) dx + \int_0^{\infty} \log(cw_0 + (1 - c)(2 - w_0)) p_t(x) dx \right] \\ &\stackrel{(ii)}{=} \arg \min_{w_0} [\log((1 - c)w_0 + c(2 - w_0)) p_t(x \leq 0) + \log(cw_0 + (1 - c)(2 - w_0)) p_t(x \geq 0)], \end{aligned}$$

where equality (i) follows from  $w_1 = 2 - w_0$  and the predictor function and (ii) follows from the fact that within each integral, the term inside the log is independent of  $x$ . Differentiating w.r.t. to  $w_0$ , we have:

$$\begin{aligned} \frac{1 - 2c}{2c + w_0 - 2cw_0} p_t(x \leq 0) + \frac{2c - 1}{2cw_0 + 2 - 2c - w_0} p_t(x \geq 0) &= 0 \\ \frac{1}{2c + w_0 - 2cw_0} p_t(x \leq 0) + \frac{-1}{2cw_0 + 2 - 2c - w_0} (1 - p_t(x \leq 0)) &= 0 \\ (2cw_0 + 2 - 2c - w_0) p_t(x \leq 0) - (2c + w_0 - 2cw_0) (1 - p_t(x \leq 0)) &= 0 \end{aligned}$$

$$2p_t(x \leq 0) - 2c - w_0 + 2cw_0 = 0,$$

which gives  $w_0 = \frac{2p_t(x \leq 0) - 2c}{1 - 2c}$ . Thus for the population MLLS estimate, the estimation error is given by

$$\|\hat{w} - w^*\| = 2|w_0 - 2\alpha| = 4 \left| \frac{(1 - 2\alpha)(p_s(x \geq 0|y = 0) - c)}{1 - 2c} \right|.$$

□

## B Proofs from Section 4

The gradient of the MLLS objective can be written as

$$\nabla_w \mathcal{L}(w, f) = \mathbb{E}_t \left[ \frac{f(x)}{f(x)^T w} \right], \quad (24)$$

and the Hessian is

$$\nabla_w^2 \mathcal{L}(w, f) = -\mathbb{E}_t \left[ \frac{f(x)f(x)^T}{(f(x)^T w)^2} \right]. \quad (25)$$

We use  $\lambda_{\min}(X)$  to denote the minimum eigenvalue of the matrix  $X$ .

**Lemma 9** (Theorem 5.1.1 [Tropp et al. \[2015\]](#)). *Let  $X_1, X_2, \dots, X_n$  be a finite sequence of identically distributed independent, random, symmetric matrices with common dimension  $k$ . Assume  $0 \preceq X \preceq R \cdot I$  and  $\mu_{\min} I \preceq \mathbb{E}[X] \preceq \mu_{\max} I$ . With probability at least  $1 - \delta$ ,*

$$\lambda_{\min} \left( \frac{1}{n} \sum_{i=1}^n X_i \right) \geq \mu_{\min} - \sqrt{\frac{2R\mu_{\min} \log(\frac{k}{\delta})}{n}}. \quad (26)$$

**Lemma 3.** *For any predictor  $f$  that satisfies Condition 1, we have*

$$\|w_f - \hat{w}_f\| \leq \sigma_{f, w_f}^{-1} \cdot \mathcal{O}_p \left( m^{-1/2} \right). \quad (12)$$

*Proof.* We present our proof in two steps. Step-1 is the non-probabilistic part, i.e., bounding the error  $\|\hat{w}_f - w_f\|$  in terms of the gradient difference  $\|\nabla_w \mathcal{L}(w_f, f) - \nabla_w \mathcal{L}_m(w_f, f)\|$ . This step uses Taylor's expansion upto second order terms for empirical log-likelihood around the true  $w^*$ . Step-2 involves deriving a concentration on the gradient difference using the Lipschitz property implied by Condition 1. Combining these two steps along with Lemma 29 concludes the proof. Now we detail each of these steps.

**Step-1.** We represent the empirical Negative Log-Likelihood (NLL) function with  $\mathcal{L}_m$  by absorbing the negative sign to simplify notation. Using a Taylor expansion, we have

$$\mathcal{L}_m(\hat{w}_f, f) = \mathcal{L}_m(w_f, f) + \langle \nabla_w \mathcal{L}_m(w_f, f), \hat{w}_f - w_f \rangle + \frac{1}{2} (\hat{w}_f - w_f)^T \nabla_w^2 \mathcal{L}_m(\tilde{w}, f) (\hat{w}_f - w_f),$$

where  $\tilde{w} \in [\hat{w}_f, w_f]$ . With the assumption  $f^T w_f \geq \tau$ , we have  $\nabla_w^2 \mathcal{L}_m(\tilde{w}, f) \geq \frac{\tau^2}{\min p_s(y)^2} \nabla_w^2 \mathcal{L}_m(w_f, f)$ .

Let  $\kappa = \frac{\tau^2}{\min p_s(y)^2}$ . Using this we get,

$$\mathcal{L}_m(\hat{w}_f, f) \geq \mathcal{L}_m(w_f, f) + \langle \nabla_w \mathcal{L}_m(w_f, f), \hat{w}_f - w_f \rangle + \frac{\kappa}{2} (\hat{w}_f - w_f)^T \nabla_w^2 \mathcal{L}_m(w_f, f) (\hat{w}_f - w_f)$$



$$\underbrace{\mathcal{L}_m(\hat{w}_f, f) - \mathcal{L}_m(w_f, f)}_I - \langle \nabla_w \mathcal{L}_m(w_f, f), \hat{w}_f - w_f \rangle \geq \frac{\kappa}{2} (\hat{w}_f - w_f)^T \nabla_w^2 \mathcal{L}_m(w_f, f) (\hat{w}_f - w_f),$$

where term-I is less than zero as  $\hat{w}_f$  is the minimizer of empirical NLL  $\mathcal{L}_m(\hat{w}_f, f)$ . Ignoring term-I and re-arranging a few terms we get:

$$-\langle \nabla_w \mathcal{L}_m(w_f, f), \hat{w}_f - w_f \rangle \geq \frac{\kappa}{2} (\hat{w}_f - w_f)^T \nabla_w^2 \mathcal{L}_m(w_f, f) (\hat{w}_f - w_f),$$

With first order optimality on  $w_f$ ,  $\langle \nabla_w \mathcal{L}(w_f, f), \hat{w}_f - w_f \rangle \geq 0$ . Plugging in this, we have,

$$\langle \nabla_w \mathcal{L}(w_f, f) - \nabla_w \mathcal{L}_m(w_f, f), \hat{w}_f - w_f \rangle \geq \frac{\kappa}{2} (\hat{w}_f - w_f)^T \nabla_w^2 \mathcal{L}_m(w_f, f) (\hat{w}_f - w_f),$$

Using Holder's inequality on the LHS we have,

$$\|\nabla_w \mathcal{L}(w_f, f) - \nabla_w \mathcal{L}_m(w_f, f)\| \|\hat{w}_f - w_f\| \geq \frac{\kappa}{2} (\hat{w}_f - w_f)^T \nabla_w^2 \mathcal{L}_m(w_f, f) (\hat{w}_f - w_f).$$

Let  $\hat{\sigma}_{f, w_f}$  be the minimum eigenvalue of  $\nabla_w^2 \mathcal{L}_m(w^*, f_c)$ . Using the fact that  $(\hat{w}_f - w_f)^T \nabla_w^2 \mathcal{L}_m(w_f, f) (\hat{w}_f - w_f) \geq \hat{\sigma}_{\min} \|\hat{w}_f - w_f\|^2$ , we get,

$$\|\nabla_w \mathcal{L}(w_f, f) - \nabla_w \mathcal{L}_m(w_f, f)\| \geq \frac{\kappa \hat{\sigma}_{f, w_f}}{2} \|\hat{w}_f - w_f\|. \quad (27)$$

**Step-2.** The empirical gradient is  $\nabla_w \mathcal{L}_m(w_f, f) = \sum_{i=1}^m \frac{\nabla_w \mathcal{L}_1(x_i, w_f, f)}{m}$  where  $\nabla \mathcal{L}_1(x_i, w_f, f) = \left[ \frac{f_1(x_i)}{\langle f(x_i), w_f \rangle} \cdots \frac{f_l(x_i)}{\langle f(x_i), w_f \rangle} \cdots \frac{f_k(x_i)}{\langle f(x_i), w_f \rangle} \right]_{(k)}$ . With the lower bound  $\tau$  on  $f^T w_f$ , we can upper bound the gradient terms as

$$\|\nabla_w \mathcal{L}_1(x, w_f, f)\| \leq \frac{\|f\|}{\tau} \leq \frac{\|f\|_1}{\tau} \leq \frac{1}{\tau}.$$

As the gradient terms decompose and are independent, using Hoeffding's inequality we have with probability at least  $1 - \frac{\delta}{2}$ ,

$$\|\nabla_w \mathcal{L}(w_f, f) - \nabla_w \mathcal{L}_m(w_f, f)\| \leq \frac{1}{2\tau} \sqrt{\frac{\log(4/\delta)}{m}}. \quad (28)$$

Let  $\sigma_{f, w_f}$  be the minimum eigenvalue of  $\nabla_w^2 \mathcal{L}(w_f, f)$ . Using lemma 9, with probability at least  $1 - \frac{\delta}{2}$ ,

$$\frac{\hat{\sigma}_{f, w_f}}{\sigma_{f, w_f}} \geq 1 - \tau \sqrt{\frac{\log(2k/\delta)}{m}}. \quad (29)$$

Plugging (28) and (29) in (27), and applying a union bound, we conclude that with probability at least  $1 - \delta$ ,

$$\begin{aligned} \|\hat{w}_f - w_f\|_2 &\leq \frac{1}{\kappa \tau} \left( \sigma_{f, w_f} - \sigma_{f, w_f} \tau \sqrt{\frac{\log(2k/\delta)}{m}} \right)^{-1} \left( \sqrt{\frac{\log(4/\delta)}{m}} \right) \\ &\leq \frac{1}{\kappa \tau} \frac{1}{\sigma_{f, w_f}} \left( 1 + \tau \sqrt{\frac{\log(2k/\delta)}{m}} \right) \sqrt{\frac{\log(4/\delta)}{m}}. \end{aligned}$$

Neglecting the order  $m$  term and letting  $c = \frac{1}{\kappa \tau}$ , we have

$$\|\hat{w}_f - w_f\| \leq \frac{c}{\sigma_{f, w_f}} \sqrt{\frac{\log(4/\delta)}{m}}.$$

□

**Lemma 4.** For any predictor  $f$  and any calibrated predictor  $f_c$  that satisfies Condition 1, we have

$$\|w_f - w^*\| \leq \sigma_{f,w^*}^{-1} \cdot C \cdot \mathbb{E}_t [\|f - f_c\|], \quad (13)$$

for some constant  $C$ .

If we set  $f_c(x) = p_s(y|f(x))$ , which is a calibrated predictor according to Proposition 3, we can further bound the error in terms of the calibration error of  $f$ <sup>8</sup>:

$$\|w_f - w^*\| \leq \sigma_{f,w^*}^{-1} \cdot C \cdot \mathcal{E}(f). \quad (14)$$

*Proof.* We present our proof in two steps. Note, all calculations are non-probabilistic. Step-1 involves bounding the error  $\|w_f - w^*\|$  in terms of the gradient difference  $\|\nabla_w \mathcal{L}(w^*, f_c) - \nabla_w \mathcal{L}(w^*, f)\|$ . This step uses Taylor's expansion on  $\mathcal{L}(w_f, f)$  upto the second order term for population log-likelihood around the true  $w^*$ . Step-2 involves deriving a bound on the gradient difference in terms of the difference  $\|f - f_c\|$  using the Lipschitz property implied by Condition 1. Further, for a crude calibration choice of  $f_c(x) = p_s(\cdot|x)$ , the gradient difference can be bounded by miscalibration error. We now detail both of these steps.

**Step-1.** Similar to Lemma 3, we represent with  $\mathcal{L}$  by absorbing the negative sign to simplify notation. Using the Taylor expansion, we have

$$\mathcal{L}(w_f, f) \geq \mathcal{L}(w^*, f) + \langle \nabla_w \mathcal{L}(w^*, f), w_f - w^* \rangle + \frac{1}{2} (w_f - w^*)^T \nabla_w^2 \mathcal{L}(\tilde{w}, f) (w_f - w^*),$$

where  $\tilde{w} \in [w_f, w^*]$ . With the assumption  $f^T w^* \geq \tau$ , we have  $\nabla_w^2 \mathcal{L}(\tilde{w}, f) \geq \frac{\tau^2}{\min p_s(y)^2} \nabla_w^2 \mathcal{L}(w^*, f)$ . Let  $\kappa = \frac{\tau^2}{\min p_s(y)^2}$ . Using this we get,

$$\begin{aligned} \mathcal{L}(w_f, f) &\geq \mathcal{L}(w^*, f) + \langle \nabla_w \mathcal{L}(w^*, f), w_f - w^* \rangle + \frac{\kappa}{2} (w_f - w^*)^T \nabla_w^2 \mathcal{L}(w^*, f) (w_f - w^*) \\ \underbrace{\mathcal{L}(w_f, f) - \mathcal{L}(w^*, f)}_{\text{I}} &\geq \langle \nabla_w \mathcal{L}(w^*, f), w_f - w^* \rangle + \frac{\kappa}{2} (w_f - w^*)^T \nabla_w^2 \mathcal{L}(w^*, f) (w_f - w^*), \end{aligned}$$

where term-I is less than zero as  $w_f$  is the minimizer of NLL  $\mathcal{L}(w, f)$ . Ignoring that term and re-arranging a few terms we get

$$-\langle \nabla_w \mathcal{L}(w^*, f), w_f - w^* \rangle \geq \frac{\kappa}{2} (w_f - w^*)^T \nabla_w^2 \mathcal{L}(w^*, f) (w_f - w^*).$$

With first order optimality on  $w^*$ ,  $\langle \nabla_w \mathcal{L}(w^*, f_c), w_f - w^* \rangle \geq 0$ . Using this we have:

$$\langle \nabla_w \mathcal{L}(w^*, f_c), w_f - w^* \rangle - \langle \nabla_w \mathcal{L}(w^*, f), w_f - w^* \rangle \geq \frac{\kappa}{2} (w_f - w^*)^T \nabla_w^2 \mathcal{L}(w^*, f) (w_f - w^*),$$

$$\langle \nabla_w \mathcal{L}(w^*, f_c) - \nabla_w \mathcal{L}(w^*, f), w_f - w^* \rangle \geq \frac{\kappa}{2} (w_f - w^*)^T \nabla_w^2 \mathcal{L}(w^*, f) (w_f - w^*).$$

As before, let  $\sigma_{f,w}$  be the minimum eigenvalue of  $\nabla_w^2 \mathcal{L}(w^*, f)$ . Using the fact that  $(w_f - w^*)^T \nabla_w^2 \mathcal{L}(w^*, f) (w_f - w^*) \geq \sigma_{f,w} \|w_f - w^*\|^2$ , we get

$$\langle \nabla_w \mathcal{L}(w^*, f_c) - \nabla_w \mathcal{L}(w^*, f), w_f - w^* \rangle \geq \frac{\kappa \sigma_{f,w}}{2} \|w_f - w^*\|^2.$$

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<sup>8</sup>We present two upper bounds because the second is more interpretable while the first is tighter.

Using Holder's inequality on the LHS and re-arranging terms gives

$$\|\nabla_w \mathcal{L}(w^*, f_c) - \nabla_w \mathcal{L}(w^*, f)\| \geq \frac{\kappa \sigma_{f,w}}{2} \|w_f - w^*\|. \quad (30)$$

**Step-2.** By lower bound assumptions  $f_c^T w^* \geq \tau$  and  $f^T w^* \geq \tau$ , we have

$$\|\nabla_w \mathcal{L}(w^*, f_c) - \nabla_w \mathcal{L}(w^*, f)\| \leq \mathbb{E}_t [\|\nabla \mathcal{L}_1(x, w^*, f_c) - \nabla \mathcal{L}_1(x, w^*, f)\|] \leq \frac{1}{\tau^2} \mathbb{E}_t [\|f_c(x) - f(x)\|], \quad (31)$$

where the first inequality is implied by Jensen's inequality and the second is implied by the Lipschitz property of the gradient. Further, we have

$$\begin{aligned} \mathbb{E}_t [\|f_c(x) - f(x)\|] &= \mathbb{E}_s \left[ \frac{p_t(x)}{p_s(x)} \|f_c(x) - f(x)\| \right] \\ &\leq \mathbb{E}_s \left[ \max_y \frac{p_t(y)}{p_s(y)} \|f_c(x) - f(x)\| \right] \\ &\leq \max_y \frac{p_t(y)}{p_s(y)} \mathbb{E}_s [\|f_c(x) - f(x)\|]. \end{aligned} \quad (32)$$

Combining equations (30), (31), and (32), we have

$$\|w_f - w^*\| \leq \frac{2}{\kappa \sigma_{f,w} \tau^2} \max_y \frac{p_t(y)}{p_s(y)} \mathbb{E}_s [\|f_c(x) - f(x)\|]. \quad (33)$$

Further, if we set  $f_c(x) = p_s(\cdot | f(x))$ , which is a calibrated predictor according to Proposition 3, we can bound the error on the RHS in terms of the calibration error of  $f$ . Using Jensen's inequality, we get

$$\mathbb{E}_s \|f_c(x) - f(x)\| \leq \left( \mathbb{E}_s \|f_c(x) - f(x)\|^2 \right)^{\frac{1}{2}} = \mathcal{E}(f). \quad (34)$$

□

**Proposition 4.** For any  $w \in \mathcal{W}$ , we have  $\sigma_{f,w} \geq p_{s,\min} \sigma_f$  where  $\sigma_f$  is the minimum eigenvalue of  $\mathbb{E}_t [f(x)f(x)^T]$  and  $p_{s,\min} = \min_{y \in \mathcal{Y}} p_s(y)$ . Furthermore, if  $f$  satisfies Condition 1, we have

$$p_{s,\min}^2 \cdot \sigma_f \leq \sigma_{f,w} \leq \tau^{-2} \cdot \sigma_f \quad (16)$$

for  $w \in \{w_f, w^*\}$ .

*Proof.* For any  $v \in \mathbb{R}^k$ , we have

$$v^T (-\nabla_w^2 \mathcal{L}(w, f)) v = \mathbb{E}_t \left[ \frac{(v^T f(x))^2}{(f(x)^T w)^2} \right] \in \left[ \frac{1}{a^2}, \frac{1}{b^2} \right] \cdot v^T \mathbb{E}_t [f(x)f(x)^T] v,$$

where

$$a = \max_{x: p_s(x) > 0} f(x)^T w \leq \frac{1}{p_{s,\min}}$$

and

$$b = \min_{x: p_s(x) > 0} f(x)^T w \geq \tau$$

if  $f$  satisfies Condition 1 and  $w \in \{w_f, w^*\}$ . Therefore, we have

$$p_{s,\min}^2 \cdot \sigma_f \leq \sigma_{f,w} \leq \tau^{-2} \cdot \sigma_f$$

for  $w \in \{w_f, w^*\}$ .

□

**Lemma 5.** Let  $f = g \circ \hat{f}$  be the predictor after post-hoc calibration with squared loss  $l$  and  $g$  belongs to a function class  $\mathcal{G}$  that satisfies the standard regularity conditions, we have

$$\mathcal{E}(f) \leq \min_{g \in \mathcal{G}} \mathcal{E}(g \circ \hat{f}) + \mathcal{O}_p \left( n^{-1/2} \right). \quad (17)$$

*Proof.* Assume regularity conditions on the model class  $\mathcal{G}_\theta$  (injectivity, Lipschitz-continuity, twice differentiability, non-singular Hessian, and consistency) as in Theorem 5.23 of Stein [1981] hold true. Using the injectivity property of the model class as in Kumar et al. [2019], we have for all  $g_1, g_2 \in \mathcal{G}$ ,

$$\text{MSE}(g_1) - \text{MSE}(g_2) = \mathcal{E}(g_1)^2 - \mathcal{E}(g_2)^2. \quad (35)$$

Let  $\hat{g}, g^* \in \mathcal{G}$  be models parameterized by  $\hat{\theta}$  and  $\theta^*$ , respectively. Using the strong concavity of the empirical mean squared error we have,

$$\text{MSE}_n(\hat{g}) \leq \text{MSE}_n(g^*) + \langle \nabla_\theta \text{MSE}_n(g^*), \hat{\theta} - \theta^* \rangle - \frac{\mu^2}{2} \|\hat{\theta} - \theta^*\|_2^2,$$

where  $\mu$  is the parameter constant for strong concavity. Re-arranging a few terms, we have

$$\frac{\mu^2}{2} \|\hat{\theta} - \theta^*\|_2^2 \leq \underbrace{\text{MSE}_n(g^*) - \text{MSE}_n(\hat{g})}_{\text{I}} + \langle \nabla_\theta \text{MSE}_n(g^*), \hat{\theta} - \theta^* \rangle,$$

where term-I is less than zero because  $\hat{g}$  is the empirical minimizer of the mean-squared error. Ignoring term-I, we get:

$$\frac{\mu^2}{2} \|\hat{\theta} - \theta^*\|_2^2 \leq \langle \nabla_\theta \text{MSE}_n(g^*), \hat{\theta} - \theta^* \rangle \leq \|\nabla_\theta \text{MSE}_n(g^*)\| \|\hat{\theta} - \theta^*\|.$$

As the assumed model class is Lipschitz w.r.t.  $\theta$ , the gradient is bounded by Lipschitz constant  $L = c_1$ .  $\mathbb{E}[\nabla_\theta \text{MSE}_n(g^*)] = 0$  as  $g^*$  is the population minimizer. Using Hoeffding's bound for bounded functions, we have with probability at least  $1 - \delta$ ,

$$\|\hat{\theta} - \theta^*\|_2 \leq \frac{c_1}{\mu^2} \sqrt{\frac{\log(2/\delta)}{n}}. \quad (36)$$

Using the smoothness of the  $\text{MSE}(g)$ , we have

$$\text{MSE}(\hat{g}) - \text{MSE}(g^*) \leq c_2 \|\hat{\theta} - \theta^*\|_2^2, \quad (37)$$

where  $c_2$  is the operator norm of the  $\nabla^2 \text{MSE}(g^*)$ . Combining (35), (36), and (37), we have for some universal constant  $c = \frac{c_1 c_2}{\mu^2}$  with probability at least  $1 - \delta$ ,

$$\mathcal{E}(\hat{g})^2 - \mathcal{E}(g^*)^2 \leq c \frac{\log(2/\delta)}{n}.$$

□

Moreover, with Lemma 4, depending on the degree of the miscalibration and the method involved to calibrate, we can bound the  $\mathcal{E}(f)$ . For example, if using vector scaling on a held out training data for calibration, we can use Lemma 5 to bound the calibration error  $\mathcal{E}(f)$ , i.e., with probability at least  $1 - \delta$ , we have

$$\mathcal{E}(f) \leq \sqrt{\min_{g \in \mathcal{G}} \mathcal{E}(g \circ f)^2 + c \frac{\log(2/\delta)}{n}} \leq \min_{g \in \mathcal{G}} \mathcal{E}(g \circ f) + \sqrt{c \frac{\log(2/\delta)}{n}}. \quad (38)$$

Plugging (34) and (38) into (33), we have with probability at least  $1 - \delta$  that

$$\|w_f - w^*\| \leq \frac{1}{\kappa \sigma_{f,w} \tau^2} \left( \|w^*\|_2 \left( \sqrt{c \frac{\log(2/\delta)}{n}} + \min_{g \in \mathcal{G}} \mathcal{E}(g \circ f) \right) \right).$$