Trustworthy Deep Learning via Proper Calibration Errors: A Unifying Approach for Quantifying the Reliability of Predictive Uncertainty

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Abstract

With model trustworthiness being crucial for sensitive real-world applications, practitioners are putting more and more focus on evaluating deep neural networks in terms of uncertainty calibration. Calibration errors are designed to quantify the reliability of probabilistic predictions but their estimators are usually biased and inconsistent. In this work, we introduce the framework of proper calibration errors, which relates every calibration error to a proper score and provides a respective upper bound with optimal estimation properties. This upper bound allows us to reliably estimate the calibration improvement of any injective recalibration method in an unbiased manner. We demonstrate that, in contrast to our approach, the most commonly used estimators are substantially biased with respect to the true improvement of recalibration methods.

1 Introduction

Deep learning became a dominant cornerstone of machine learning research in the last decade and deep neural networks can surpass human-level predictive performance on a wide range of tasks [1,2,3]. However, Guo et al. 2017 [4] have shown that for modern neural networks with higher capacity, better classification accuracy can come at the cost of systematic overconfidence in their predictions. Practitioners in sensitive forecasting domains, such as cancer diagnostics [3], genotype-based disease prediction [5] or climate prediction [6], require for models to not only have high predictive power but also to reliably communicate uncertainty. This raises the need to quantify the quality of predictive uncertainty, ideally via a dedicated metric. An uncertainty-aware model should give probabilistic predictions which represent the true likelihood of events depending on the very prediction. To quantify the extend to which this condition is violated, calibration errors have been introduced. In general, these errors are intractable to compute, and estimators are usually heavily biased and inconsistent [7]. This, in turn, is highly problematic since we cannot quantify how reliable a model is if we do not know how reliable the metric is. The bias of the estimators is a concern especially in low data regimes occurring, for example, in the medical domain with low expert availability and/or disease frequency - which is a domain that also requires high model trustworthiness. Resampling strategies can be viable options for optimization on small datasets, but the reduced evaluation set sizes further lower the reliability of calibration estimates.

Since deep neural networks typically only yield uncalibrated confidence scores, a variety of different post-hoc recalibration approaches have been proposed [9,10]. These methods use the validation set to transform predictions returned by a trained neural network such that they become better calibrated.

A key desired property of recalibration methods is to not reduce the accuracy after the transformation. Therefore, most modern approaches are restricted to accuracy preserving transformations of the model outputs [11,12,13]. When recalibrating a model, it is crucial that a reliable estimate of how much the chosen method improves the underlying model is available. However, when using current estimators for calibration errors, their biased nature results in estimates that are highly sensitive to the number of samples in the test set that are used to compute the calibration error before and after recalibration (Fig. 1; c.f. section 5).
Our contributions towards reliably quantifying uncertainty calibration are summarized in the following. We...

• ... give an overview of current calibration error literature, place the errors into a taxonomy, and show which are insufficient for calibration quantification. This also includes a chain of inequalities, which is dominated by the Brier score.

• ... introduce the framework of proper calibration errors, which gives important guarantees and relates every element to a proper score. We can reliably estimate the improvement of an injective recalibration method w.r.t. a proper calibration error via its related proper score.

• ... show that common calibration estimators are highly sensitive w.r.t. the test set size. We demonstrate that for all previously proposed estimators, the estimated improvement of recalibration methods is heavily biased and the estimated calibration improvement becomes monotonically worse with fewer test data.

2 Related Work

In this section, we give an extensive overview of published work regarding quantifying model calibration and model recalibration. The presented definitions will be the basis for our theoretical findings. These will motivate the definition of proper calibration errors, which are directly related to proper scores. Consequently, we will also present important aspects of the framework around proper scores in later parts of this section.

2.1 Calibration errors

A systematic overview of the multitude of calibration errors proposed in the recent literature requires a common notation that can be used to harmonize definitions. For the sake of clarity, we use formulations close to the notation introduced in [10] and adjust the other errors accordingly, while retaining the notation of the original work whenever possible. Assume we have random variables $X$ and $Y$ corresponding to feature and target variable, and feature and target space $\mathcal{X}$ and $\mathcal{Y}$. We have $P_Y, P_{Y|X} \in \mathcal{P}$, where $P_Y$ refers to the distribution of $Y$, $P_{Y|X}$ to the conditional distribution given $X$, and $\mathcal{P}$ a set of distributions on $\mathcal{Y}$. Even though some approaches explore calibration for regression tasks [14, 15, 16], it is most dominantly considered for classification.

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To distinguish between the general case and $n$-class classification, we refer to $\mathcal{P}_n$ as the $n$-dimensional simplex of corresponding categorical distributions.

A popular task is the calibration of the predicted top-label $\hat{C} = \arg \max_k f_k(X)$ of a model $f : \mathcal{X} \rightarrow \mathcal{P}_n$ [4, 17, 18, 19, 8, 20, 13]. Specifically, this is addressed via the condition $P(Y = C \mid f_C(X)) = f_C(X)$. However, this is a weaker condition as one might expect, and referring to a model fulfilling this condition as (perfectly) calibrated can give a false sense of security [8, 21]. This holds especially in forecasting domains, where low likelihood estimates can still be highly relevant. For example, assigning probability mass to an aggressive type of cancer can still trigger action even if it is not predicted as the most likely outcome. Consequently, we are in general more interested in finding a model that fulfills the stricter and more general condition in the following.

Definition 2.1. A model $f : \mathcal{X} \rightarrow \mathcal{P}$ is strongly calibrated if and only if $P_{Y|f(X)} = f(X)$.

In contrast to [21], where this definition is given for classification, our formulation covers the general case of arbitrary distributions.

One of the first metrics for assessing model calibration that is still widely used in recent literature is the Brier score (BS) [22, 11, 23, 13].
**Definition 2.2.** The expected Brier score \( [24] \) of model \( f: \mathcal{X} \rightarrow \mathcal{P}_n \) is defined as

\[
\text{BS}(f) = \mathbb{E} \left[ \| f(X) - \mathbb{P}_Y(X) \|_2^2 \right]
\]

where \( e_i \) is a vector of zeros with a ‘1’ at index \( i \).

The estimator of the BS is equivalent to the mean squared error, illustrating that it does not purely capture model calibration. Rather, the BS can be interpreted as a comprehensive measure of model performance, simultaneously capturing model fit and calibration. This becomes more obvious via the canonical decomposition of the BS into a calibration and sharpness term \([23]\). Based on this decomposition, we can derive the following calibration error.

**Definition 2.3.** The \( \ell_p \) calibration error of model \( f: \mathcal{X} \rightarrow \mathcal{P}_n \) is defined as

\[
\text{CE}_p(f) = \mathbb{E} \left[ \| f(X) - \mathbb{P}_Y|f(X) \|_p \right]
\]

for \( 1 \leq p \leq \mathbb{R} \).

The BS decomposition only supports the case \( p = 2 \), but a general \( \ell_p \) formulation became more common in recent years \([8,21,12]\).

The \( \text{CE}_p \) is intractable to reliably estimate in the general case. This is mostly due to the term \( \mathbb{P}_Y|f(X) \) since we never have samples of every possible prediction for continuous models. This is in contrast to the original work of \([22]\), where only models with a finite prediction space are considered so that computing the \( \text{CE}_2 \) does not require a special procedure. To assess the calibration of a continuous binary model Platt 1999 \([11]\) used histogram estimation, transforming the infinite prediction space to a finite one. This is also referred to as equal width binning. Similarly, Nguyen et al.\([?]\) introduced an equal mass binning scheme for continuous binary models. Both, equal width and equal mass binning schemes, suffer from the requirement of setting a hyperparameter. This can significantly influence the estimated value \([10]\) and there is no optimal default since every setting has a different bias-variance tradeoff \([19]\).

The first calibration estimator for a continuous one-vs-all multi-class model was given by \([25]\) and is still the most commonly used measure to quantify calibration. It is referred to as expected calibration error (ECE) and can be formulated in expectation as in the following.

**Definition 2.4.** The expected calibration error of model \( f: \mathcal{X} \rightarrow \mathcal{P}_n \) is defined as

\[
\text{ECE}(f) = \sum_{i=1}^{m} \mathbb{P} \left( f_C(X) \in B_i \right) \cdot \left[ \mathbb{E} \left[ f_C(X) \mid f_C(X) \in B_i \right] - \mathbb{P} \left( Y = C \mid f_C(X) \in B_i \right) \right]
\]

with top-label \( C := \arg \max_k f_k(X) \) and \( m \) bins \( B_i := \left( \frac{i-1}{m}, \frac{i}{m} \right) \), where \( m \in \mathbb{N} \) is user-defined.

We can reliably estimate \( \mathbb{E} \left[ f_C(X) \mid f_C(X) \in B_i \right] \) via the bin-conditional mean, \( \mathbb{P} \left( Y = \arg \max_k f_k(X) \in B_i \right) \) via the bin-conditional frequency, and \( \mathbb{P} \left( f_C(X) \in B_i \right) \) via the bin frequency. These are then plugged into definition \( [23]\) to estimate the ECE.

\([25]\) and \([19]\) independently introduced another calibration estimator, which also captures the extent to which the class-wise condition \( \mathbb{P} \left( Y = k \mid f_k(X) \right) = f_k(X) \) is violated. They respectively use equal width and equal mass binning.

\([27]\) showed that the plug-in estimation of the squared calibration term is biased and introduced a term for bias reduction. Based on this, \([10]\) introduced a calibration error estimator based on equal mass binning and a bias reduction procedure. We follow \([10]\) and define top-label and class-wise calibration errors in expectation:

**Definition 2.5.** The top-label calibration error of model \( f: \mathcal{X} \rightarrow \mathcal{P}_n \) is defined as

\[
\text{TCE}_p(f) = \left( \mathbb{E} \left[ f_C(X) \right] - \mathbb{P} \left( Y = C \mid f_C(X) \right) \right)^\frac{1}{p}
\]

with \( C := \arg \max_k f_k(X) \) and the class-wise calibration error is defined as

\[
\text{CWCE}_p(f) = \left( \sum_{k \in \mathbb{Y}} \mathbb{E} \left[ f_k(X) \right] - \mathbb{P} \left( Y = k \mid f_k(X) \right) \right)^\frac{1}{p}
\]

for \( 1 \leq p \leq \mathbb{R} \).

Note that we removed the weighting factors from the original definition in \([10]\) for easier comparison with the other errors and a fixed upper limit (we will show that \( \text{CWCE}_p \leq 2 \)). Furthermore, \([10]\) and \([8]\) proved independently that using a fixed binning scheme for estimation leads to a lower bound of the expected error. So, even with infinite data, such estimators systematically underestimate the true calibration error. \([12]\) circumvent binning schemes by using kernel density estimation to estimate the TCE. To compare different estimators, \([7]\) performed empirical benchmarks regarding the estimation bias and concluded that every estimator proposed so far is biased. And even though kernel density estimation does not result in a theoretical lower bound like binning schemes, its estimation bias can be significantly worse. They further introduce another binning-based estimator, which is also biased. Consequently, \([23]\) concluded that current calibration error estimators are unfit for the low data regime. In later sections, we will further demonstrate that, even if there exists a perfect estimator, the TCE and CWCE fail to quantify the extent to which a model violates condition \([2,1]\) of being strongly calibrated.

Orthogonal ways to quantify model miscalibration have been proposed to not depend on binning
or kernel density estimation schemes. [23] introduced a calibration error, which is based on the Kolmogorov-Smirnov test between empirical cumulative distribution functions. Its estimator does not require setting a hyperparameter.

**Definition 2.6.** The Kolmogorov-Smirnov calibration error [23] of model \( f: \mathcal{X} \to \mathcal{P}_n \) is given by

\[
\text{KS} (f) = \mathbb{E} [\text{KS} (f, C)],
\]

where \( C = \arg \max_k f_k (X) \) and \( \text{KS} (f, k) = \max_{\sigma \in [0, 1]} \left| \int_{[0, \sigma]} z - \mathbb{P} (Y = k | f_k (X) = z) \, dz \right| \).

Estimators of the TCE\(_n\) and CWCE\(_n\) are in general not differentiable. This motivates the introduction of the following error, for which a differentiable estimator was proposed.

**Definition 2.7.** Given a reproducing kernel Hilbert space \( \mathcal{H} \) with kernel \( k: [0, 1] \times [0, 1] \to \mathbb{R} \) the maximum mean calibration error [17] of model \( f: \mathcal{X} \to \mathcal{P}_n \) is

\[
\text{MMCE} (f) = \mathbb{E} \left[ \left| \mathbb{E} [f_C (X)] - \mathbb{P} (Y = C | f_C (X)) \right| \right] \mathcal{H}.
\]

[21] argued that the MMCE is insufficient for quantifying strong calibration of a model. They further proposed a calibration error, which is, as the MMCE, based on reproducing kernel Hilbert spaces. Unlike MMCE, which only uses the top-label prediction, it includes the whole model prediction.

**Definition 2.8.** Given a reproducing kernel Hilbert space \( \mathcal{H} \) with kernel \( k: \mathcal{P}_n \times \mathcal{P}_n \to \mathbb{R} \times \mathbb{R}^n \) the kernel calibration error [21] of model \( f: \mathcal{X} \to \mathcal{P}_n \) is

\[
\text{KCE} (f) = \mathbb{E} \left[ \left| (f (X) - \mathbb{P} (Y | f (X)) \right) \, k (f (X))) \right| \mathcal{H} .
\]

The squared KCE has an unbiased estimator based on a U-statistic. However, even though the KCE is positive, this estimator can give negative values, and the KCE lacks interpretability. These drawbacks can be circumvented by computing a p-value. To this end, the authors use the estimated value as a test statistic w.r.t. the null hypothesis that the model is strongly calibrated.

Furthermore, [21] proposed to unify different definitions of calibration errors in a theoretical framework. However, it is very broadly defined and allows for calibration errors, which are zero even if the model is not calibrated at all.

**2.2 Recalibration**

A plethora of recalibration methods have been proposed to improve model calibration after training by transforming the model output probabilities [29, 11, 30, 31, 25, 32, 33, 1, 24, 10, 12, 23, 13]. These methods are optimized on a specific calibration set, which is usually the validation set. Key desiderata of these methods include for the algorithms to be accuracy-preserving and data-efficient [12], reflecting that typical use-cases include settings in sensitive domains where accuracy should remain unchanged and often little data is available to train and evaluate the models. Such accuracy-preserving methods only adjust the probability estimate in such a way that the predicted top-label remains the same. The most commonly used accuracy-preserving recalibration method is temperature scaling (TS) [4], where the model logits are divided by a parameter \( T \in \mathbb{R} > 0 \) before computing the predictions via softmax. A more expressive extension of TS is ensemble temperature scaling (ETS) [12], where a weighted ensemble of TS output, model output, and label smoothing is computed. Recently, [13] proposed different classes of order-preserving transformations. A specifically interesting one is the class of diagonal intra order-preserving functions (DIAG). Here, the model logits are transformed elementwise with a scalar, monotonic, and continuous function, which is represented by neural networks of unconstrained monotonic functions [34].

**2.3 Proper scores**

[35] give an extensive overview of proper scores. Unfortunately, their presented definitions assume maximization as the model training objective. To stay in line with recent machine learning literature, we flip the sign when it is required in the following definitions, similar as in [35].

We specifically do not constrain ourselves to classification, which is a special case. Assume we give a prediction in \( \mathcal{P} \) for an event in \( \mathcal{Y} \) and we want to score how good the prediction was. A function \( S: \mathcal{P} \times \mathcal{Y} \to \mathbb{R} \) with \( \mathbb{R} := \mathbb{R} \cup \{-\infty, \infty\} \) is called **scoring rule** or just **score**. Examples are the Brier score or the log score. To use a score for comparing distributions, we require the following.

**Definition 2.9.** A scoring function \( s_S \) based on a scoring rule \( S \) is defined as

\[
s_S : \mathcal{P} \times \mathcal{P} \to \mathbb{R}
\]

\[
(P, Q) \mapsto \int_{\mathcal{Y}} S (P, y) \, dQ (y)
\]

If \( Q \) is the distribution of \( Y \) we can also write \( s_S (P, Q) = \mathbb{E} [S (P, Y)] \). In this case, we can call \( s_S \) the expected score and estimate it via the mean
score. For example, the cross-entropy risk is the estimator of the expected log score.

**Definition 2.10.** A scoring rule $S$ is defined to be **proper** if and only if $s_S(P, Q) \geq s_S(Q, Q)$ holds for all $P, Q \in \mathcal{P}$, and **strictly proper** if and only if $P \neq Q \implies s_S(P, Q) > s_S(Q, Q)$.

In other words, a score is proper if predicting the target distribution gives the best expected value and strictly proper if no other prediction can achieve this value.

**Definition 2.11.** Given a proper score $S$ and $P, Q \in \mathcal{P}$, the associated **divergence** is defined as

$$d_S(P, Q) = s_S(P, Q) - s_S(Q, Q)$$

and the associated **generalized entropy** as

$$g_S(Q) = s_S(Q, Q).$$

For strictly proper $S$, $d_S$ is only zero if $P = Q$; for (strictly) proper $S$, $g_S$ is (strictly) concave. Examples of divergences and generalized entropies are the Kullback-Leibler divergence and the Shannon entropy, or the squared Euclidean distance and the variance of an implied distribution.

### 3 Relationships between calibration errors

In this section, we present a taxonomy of the introduced calibration errors. At first, we compare the errors in a hierarchy before we give an example of how far errors lower in the hierarchy can differ from the CE$_2$. We illustrate the practical relevance of this analysis by introducing a perfect calibration method according to most errors. The transformed model will have zero calibration error according to these but fails to be strongly calibrated. All proofs are presented in Appendix 9.

**Theorem 3.1.** Given a model $f : \mathcal{X} \rightarrow \mathcal{P}_n$ and the above defined errors, we have

$$BS(f) = 0 \implies CE_p(f) = 0 \implies KCE(f) = 0 \implies f \text{ is strongly calibrated} \implies CWCE_p(f) = 0 \implies TCE_p(f) = 0 \implies MMCE(f) = 0 \implies KS(f) = 0 \implies ECE(f) = 0 \tag{1}$$

and

$$2^{\frac{1}{p}} \geq (BS(f))^\frac{1}{p} \geq (CE_p(f))^\frac{1}{p} \geq CWCE_p(f) \geq TCE_p(f) \geq TCE_1(f) \geq \left\{ \begin{array}{ll} KS(f) & \geq 0 \\ ECE(f) & \geq 0 \\ c \cdot MMCE(f) & \end{array} \right\} \text{ for } 1 \leq p \in \mathbb{R}. \ * BS \text{ is only included for } p = 2.$$  

No implication in (1) can be reverted in the general case. From this theorem follows that it is ambiguous to refer to perfect calibration just because there exists a calibration error which is zero for a model. We now further demonstrate how misleading improper calibration errors can be.

**Proposition 3.2.** For all $\epsilon > 0$ and surjective $f : \mathcal{X} \rightarrow \mathcal{P}_n$ there exists a joint distribution $\mathbb{P}_{XY}$ such that for all $E \in \{MMCE, KS, ECE, TCE_p, CWCE_p | 1 \leq p \in \mathbb{R} \}$:

$$E(f) = 0 \land CE_2(f) \geq 1 - \frac{1}{n} - \epsilon.$$

E.g. for binary classification and $\epsilon = 0.01$, we have $CE_2(f) \geq 0.49$. We also have $CE_2(f) = 0$ if and only if $f$ is strongly calibrated. In other words, most used calibration errors can be zero, but the model is still far from strongly calibrated. Furthermore, this questions the reliability of reliability diagrams since they correspond to either ECE, TCE$_p$, CWCE$_p$, or KS.

**Proposition 3.3.** For all models $f : \mathcal{X} \rightarrow \mathcal{P}_n$ and $E \in \{MMCE, KS, ECE, TCE_p | 1 \leq p \in \mathbb{R} \}$ we have

$$E(t^f \circ f) = 0 \land ACC(t^f \circ f) = ACC(f).$$

But, in general $CE_p(t^f \circ f) > 0$.  

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Propositions 3.2 and 3.3 motivate the formal definition of a framework of proper calibration errors which are zero if and only if the model is strongly calibrated (c.f. Definition 2.1).

4 Proper calibration errors

In this section, we introduce the definition of proper calibration errors. We provide an easy-to-estimate upper bound and investigate some properties. As a preliminary step, we generalize a proper score decomposition. Again, all proofs are presented in Appendix 9. We introduced a calibration-sharpness decomposition of proper scores w.r.t. categorical distributions. We extend this decomposition to proper scores of arbitrary distributions.

Lemma 4.1. Let \( \mathcal{P} \) be a set of arbitrary distributions for which exists a proper score \( S \) with some mild conditions. For random variables \( Q \) and \( Y \) with \( Q, P_Y, P_{Y|X} \in \mathcal{P} \), we have the decomposition

\[
E[S(Q,Y)] = E[g_S(P_Y) - E[d_S(P_Y, P_{Y|Q})] + E[d_S(Q, P)]]
\]

A familiar example would be the cross-entropy, which decomposes into Shannon entropy minus mutual information plus Kullback-Leibler based calibration (see table 1). Substituting \( Q \) with \( f(X) \) and \( S \) with the Brier score, the calibration term equals the previously defined CE2 of a model \( f \).

Lemma 4.1 motivates the following definition, which we introduce:

**Definition 4.2.** Given a model \( f : \mathcal{X} \to \mathcal{P} \), we say

\[
\text{CE}_S(f) \doteq E[d_S(f(X), P_{Y|f(X)})]
\]

is a (strictly) proper calibration error if and only if \( d_S \) is a divergence associated with a (strictly) proper score \( S \).

This gives CEBS \( \equiv \text{CE} \) as an example of a strictly proper calibration error for classification since the Brier score is a strictly proper score on \( \mathcal{P}_n \). Strictly proper calibration errors have the highly desired property: \( \text{CE}_S(f) = 0 \) if and only if \( f \) is strongly calibrated. Since proper scores are not restricted to classification, the above definition gives a natural extension of calibration errors beyond classification.

Additionally, by generalizing the definition of proper scores, we can show that the squared KCE is a strictly proper calibration error (Appendix 11). But, in general, there does not exist an unbiased estimator of a proper calibration error, since we cannot estimate \( E[g_S(P_{Y|f(X)})] \) in an unbiased manner. Because we do not want lower bounds for errors used in sensitive applications, we introduce the following theorem about how to construct an upper bound.

**Theorem 4.3.** For all proper calibration errors with \( \inf_{P \in \mathcal{P}} g_S(P) \in \mathbb{R} \), there exists an associated calibration upper bound

\[
\mathcal{U}_S(f) \geq \text{CE}_S(f)
\]

defined as \( \mathcal{U}_S(f) = E[S(f(X), Y)] - \inf_{P \in \mathcal{P}} g_S(P) \). Under a classification setting and further mild conditions, we have \( \lim_{\mathcal{ACC}(f) \to 1} \mathcal{U}_S(f) - \text{CE}_S(f) = 0 \).

In other words, we can always construct a non-trivial upper bound of a proper calibration error as long as the generalized entropy function has a finite infimum. The calibration upper bound approaches the true calibration error for models with high accuracy. For the Brier score we have \( \inf_{P \in \mathcal{P}} g_{BS}(P) = 0 \), making the Brier score itself an upper bound of its induced calibration error. In table 1 we give an overview of the most prominent scores, their calibration errors, and calibration upper bounds.

Our proposed calibration upper bounds are provably reliable to use since they all have a minimum-variance unbiased estimator. Theorem 3.1 states \( \sqrt{BS(f)} \geq \text{TCE}_E(f) \geq ECE(f) \). Consequently, we might also be interested in transforming the estimated upper bound in a non-linear way for interpretability purposes. In general, any unbiased estimator \( \hat{\theta} \) becomes biased after a non-linear transformation \( t \), since \( E[t(\hat{\theta})] \neq t(E[\hat{\theta}]) \). But, if \( t \) is continuous, our estimator is still asymptotically...
unbiased and consistent [37]. This means that an empirical robustness w.r.t. data size indicates a neglectable bias for finite data. We will further investigate this in section 5.

Furthermore, $\mathcal{V}_S$ has the following properties, which are helpful for the application of recalibration method optimization and selection.

**Proposition 4.4.** Given injective functions $h, h' : \mathcal{P} \to \mathcal{P}$ we have

$$\mathcal{V}_S(h \circ f) - \mathcal{V}_S(f) = CE_S(h \circ f) - CE_S(f),$$

$$\mathcal{V}_S(h \circ f) > \mathcal{V}_S(h' \circ f) \iff CE_S(h \circ f) > CE_S(h' \circ f)$$

and (assuming $S$ is differentiable)

$$\frac{d\mathcal{V}_S(h \circ f)}{dh} = \frac{dCE_S(h \circ f)}{dh}.$$

This is a generalization of Proposition 4.2 presented in [12]. It tells us that we can reliably estimate the improvement of any injective recalibration method via the upper bound. Furthermore, we get access to the calibration gradient and can compare different transformations. At first, injectivity seems like a significant restriction. But, we argue in the following that injectivity - rather than being accuracy-preserving - is a desired property of general recalibration methods. For example, we can construct a recalibration method, which is strongly calibrated and accuracy-preserving, but only predicts a finite set of distinct values (see Appendix 10). Specifically, we would only predict two distinct values for any input in binary classification. To exclude such naive solutions which substantially reduce model sharpness, we restrict ourselves to injective transformations of $\mathcal{P}_n \to \mathcal{P}_n$. These do provably not impact the model sharpness and preserve, at least partly, the continuity of the output space. Examples of injective transformations are TS, ETS, and DIAG. These state-of-the-art methods show very competitive performances even when compared to non-injective recalibration methods [12, 13].

5 Experiments

In the following, we investigate the behavior of calibration error estimators in two key settings. First, we use varying test set sizes for the estimators and compare their values. This will show how well the inequalities in Theorem 3.1 hold in practical settings and how robust the estimators are. Second, we explore what the estimated improvements of several recalibration methods are. This is done after the recalibration methods are already optimized on a given validation set; we only vary the size of the test set and compute calibration errors on these test sets before and after recalibration. In both settings, the straighter a line is, the more robust and, consequently, trustworthy is the estimator for practical applications.

In all experiments we evaluate the following estimators: CWCE$_2$ with 15 equal width bins (‘15b CWCE$_2$’), CWCE$_2$ with 100 equal width bins (‘100b CWCE$_2$’), ECE with 15 equal width bins (‘ECE’), TCE$_2$ with 100 equal width bins (‘100b TCE$_2$’), TCE$_2$ with 15 mass bins and debias term (‘15b d TCE$_2$’), TCE$_2$ with kernel density estimation (‘KDE TCE$_2$’), KS (‘KS’) and the root calibration upper bound $\sqrt{\mathcal{V}_S(f)}$ (‘RBS (ours)’). We exclude MMCE and KCE since they are not directly comparable with the other errors. The experiments are conducted across several model-dataset combinations, for which logit sets are openly accessible [26, 13]. This includes the models Wide ResNet 32 [32], DenseNet 40, and DenseNet 161 [39] and the datasets CIFAR10, CIFAR100 [40], and ImageNet [11]. We did not conduct model training ourselves and refer to [26] and [13] for further details. We include TS, ETS, and DIAG as injective recalibration methods. Further details and results on additional models and datasets are reported in the Appendix 12.

**Robustness of calibration errors to test set size** We first illustrate the estimated values of our introduced upper bound and the other errors, which are lower bounds of the unknown CE$_2$ (first row of figure 3). All values represent the calibration of the given model without recalibration transformation. Only our proposed upper bound and KS are stable across a wide range of test set sizes in different settings. The theoretically highest lower bound (CWCE$_2$ with 100 bins) is also constantly the highest estimated lower bound, but it is sensitive to the test set size. We further illustrate this

| Score | $CE_S(f)$ | $\mathcal{V}_S(f)$ |
|-------|----------|------------------|
| BRIER | $E \left[ \| f(X) - P_{Y \mid f(X)} \|^2 \right]$ | $E \left[ \| f(X) - eY \|^2 \right]$ |
| LOG   | $E \left[ D_{KL}(f(X), P_{Y \mid f(X)}) \right]$ | $E \left[ -\log P_Y(X) \right]$ |
sensitivity by aggregating the respective calibration errors for DenseNet 40, Wide ResNet 32, ResNet 110 SD, ResNet 110, and LeNet 5 trained on CIFAR10 and show the relative change in calibration error w.r.t. the full test set size (Fig. 2). Results for further settings presented in Appendix 12 show similar results.

Quantifying recalibration improvement
Next, we assessed how well all estimators were able to quantify the improvement in calibration error after applying different injective recalibration methods (Fig. 1, 3 bottom). Only our proposed upper bound estimator RBS is again robust throughout all settings. According to Proposition 4.4 and since RBS is asymptotically unbiased and consistent, it can be regarded as a reliable approximation of the real improvement of the recalibration methods. For all other estimators, there is a general trend to estimate recalibration improvement higher for large test set sizes. In other settings, especially for small test set sizes, calibration improvement is underestimated to the extent that negative improvements (poorer calibration than before) are suggested. Results on other settings presented in Appendix 12 show similar results. Taken together, these experiments demonstrate the unreliability of existing calibration estimators, in particular, when used to evaluate recalibration methods. In contrast, our proposed upper bound estimator is stable across different settings.

6 Conclusion
In this work, we address the problem of reliably quantifying uncertainty calibration. To this end, we first provide harmonized definitions of existing calibration errors for DenseNet 40, Wide ResNet 32, ResNet 110 SD, ResNet 110, and LeNet 5 trained on CIFAR10 and show the relative change in calibration error w.r.t. the full test set size (Fig. 2). Results for further settings presented in Appendix 12 show similar results. Taken together, these experiments demonstrate the unreliability of existing calibration estimators, in particular, when used to evaluate recalibration methods. In contrast, our proposed upper bound estimator is stable across different settings.
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7 Appendix

In this appendix we

- Introduce some notation in section 8 that we will use throughout the appendix.
- Provide proofs for all claims that we make in the main text in section 9.
- Provide details on several recalibration transformations that we introduced in the main text to illustrate the shortcomings of existing approaches (section 10).
- Give a detailed overview of proper U-scores that can be used to further generalize our proposed framework of proper calibration errors (section 11).
- Give more experimental details and report results from additional experiments (section 12).

8 Notation

The following is implied throughout the appendix. We will use

- The underlying probability space $(\Omega, \mathcal{F}, \mathbb{P})$, $\mathcal{X}$ the feature space, and $\mathcal{Y}$ the target space.
- Random variables $X: \Omega \to \mathcal{X}$ and $Y: \Omega \to \mathcal{Y}$.
- $\mathbb{P}_{Y|X=x}(y) := \frac{\mathbb{P}(\omega \in \Omega | X(\omega) = x, Y(\omega) = y)}{\mathbb{P}(\omega \in \Omega | X(\omega) = x)}$ and $\mathbb{P}_Y(y) := \mathbb{P}(\{\omega \in \Omega | Y(\omega) = y\})$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$.
- $\mathcal{P}_n, \mathbb{P}_{Y|X=x} \in \mathcal{P}_n$ with $\mathcal{P}_n = \{p \in [0,1]^n | \sum_k p_k = 1\}$, and $\mathcal{Y} = \{1, \ldots, n\}$ for categorical $Y$ with $n \in \mathbb{N}$ classes.
- The index ‘−k’ on a finite vector to denote the removal of index $k$.
- The random variable $C: \Omega \to \mathcal{Y}$ defined as $C := \arg \max_k f_k(X)$ for $f: \mathcal{X} \to \mathcal{P}_n$. It can be regarded as the top-label prediction of $f$.

The notation regarding the (conditional) probability measures will be used for arbitrary random variables.

9 Proofs

9.1 Helpers

The following will be of use in several proofs.

**Lemma 9.1.** Assume that $S$ is a proper score for which $CE_S$ exists, then we have

$$CE_S(f) = \mathbb{E}[S(f(X), Y)] - \mathbb{E} [gs (\mathbb{P}_{Y|f(X)})].$$

**Proof.**

$$CE_S(f) \overset{\text{def}}{=} \mathbb{E} [d_{S} (f(X), \mathbb{P}_{Y|f(X)})]
\overset{\text{def}}{=} \mathbb{E} [s_{S} (f(X), \mathbb{P}_{Y|f(X)}) - s_{S} (\mathbb{P}_{Y|f(X)}, \mathbb{P}_{Y|f(X)})]
\overset{\text{def}}{=} \mathbb{E} [s_{S} (f(X), \mathbb{P}_{Y|f(X)})] - \mathbb{E} [gs (\mathbb{P}_{Y|f(X)})]
= \int s_{S} (z, \mathbb{P}_{Y|f(X)} = z) \, d\mathbb{P}_{f(X)}(z) - \mathbb{E} [gs (\mathbb{P}_{Y|f(X)})]
= \int S(z, y) \, d\mathbb{P}_{Y|f(X)}(y, z) - \mathbb{E} [gs (\mathbb{P}_{Y|f(X)})]
= \mathbb{E} [S(f(X), Y)] - \mathbb{E} [gs (\mathbb{P}_{Y|f(X)})].\quad (3)$$

\[\square\]
9.2 Theorem 3.1

Given a model \( f : \mathcal{X} \to \mathcal{P}_n \) and the above defined errors, we have

\[
\text{BS}(f) = 0 \quad \Rightarrow \quad \text{CE}_p(f) = 0 \quad \Leftrightarrow \quad \text{KCE}(f) = 0
\]

\( \Leftrightarrow \) \( f \) is strongly calibrated

\( \Rightarrow \) \( \text{CWCE}_p(f) = 0 \)

\( \Rightarrow \) \( \text{TCE}_p(f) = 0 \)

\( \Rightarrow \) \( \text{MMCE}(f) = 0 \)

\( \Leftrightarrow \) \( \text{KS}(f) = 0 \)

\( \Rightarrow \) \( \text{ECE}(f) = 0 \)

(4)

and

\[
2^\frac{1}{p} \geq \left( \text{BS}(f) \right)^{\frac{1}{p}} \\
\geq \left( \text{CE}_p(f) \right)^{\frac{1}{p}} \\
\geq \text{CWCE}_p(f) \\
\geq \text{TCE}_p(f) \\
\geq \text{TCE}_1(f) \\
\geq \begin{cases} 
\text{KS}(f) \\
\text{ECE}(f) \\
c \cdot \text{MMCE}(f) 
\end{cases} \geq 0
\]

(5)

for \( 1 \leq p \in \mathbb{R} \). * BS is only included for \( p = 2 \). We define \( c = (\max_r k(r,r))^{-\frac{1}{2}} \) as given in Theorem 3 of [17].

**Proof.** Regarding \( \text{BS}(f) = 0 \Rightarrow \text{CE}_p(f) = 0 \Leftrightarrow \text{KCE}(f) = 0 \Leftrightarrow f \) is strongly calibrated:

\[
\text{BS}(f) = 0 \Leftrightarrow \mathbb{P}_{Y|X} \overset{a.s.}{=} f(X) \\
\Rightarrow \mathbb{P}_{Y|f(X)} \overset{a.s.}{=} f(X) \\
\Leftrightarrow \begin{cases} 
\text{CE}_p(f) = 0 \\
\text{KCE}(f) = 0 \\
f \text{ is strongly calibrated}
\end{cases}
\]

(6)

The last equivalence follows from Definition 2.1 and 2.3, and according to [21]. Since the equivalence in the last line holds for each, it follows \( \text{CE}_p(f) = 0 \Leftrightarrow \text{KCE}(f) = 0 \Leftrightarrow f \) is strongly calibrated. Example sketch for \( \text{BS}(f) = 0 \Leftrightarrow \text{CE}_p(f) = 0 \) is given in Proposition 3.2.

Regarding \( \text{CE}_p(f) = 0 \Rightarrow \text{CWCE}_p(f) = 0 \):

\[
\text{CE}_p(f) = 0 \Leftrightarrow \mathbb{P}_{Y|f(X)} \overset{a.s.}{=} f(X) \\
\Leftrightarrow \mathbb{P}(Y = k \mid f(X)) \overset{a.s.}{=} f_k(X) \quad \forall k \\
\Rightarrow \mathbb{E}_{f_k(X)}[\mathbb{P}(Y = k \mid f(X)) - f_k(X)] \overset{a.s.}{=} \mathbb{E}_{f_k(X)}[f_k(X) - f_k(X)] \quad \forall k \\
\Rightarrow \mathbb{P}(Y = k \mid f_k(X)) - f_k(X) \overset{a.s.}{=} f_k(X) \quad \forall k \\
\Leftrightarrow \sum_{k \in \mathcal{Y}} \mathbb{E}[(\mathbb{P}(Y = k \mid f_k(X)) - f_k(X))^2] = 0 \\
\Leftrightarrow \text{CWCE}_p(f) = 0
\]

(7)

An example for \( \text{CE}_p(f) = 0 \Leftrightarrow \text{CWCE}_p(f) = 0 \) is given in Proposition 3.2.
Regarding CWCE\(_p\) \((f) = 0 \iff \text{TCE}_p\) \((f) = 0 \iff \text{MMCE}(f) = 0\):

\[
\text{CWCE}_p\) \((f) = 0 \iff P(Y = k \mid f_k(X)) \overset{a.s.}{=} f_k(X) \quad \forall k
\]

\[
\implies \ P(Y = C \mid f_C(X)) \overset{a.s.}{=} f_C(X)
\]

\[
\iff \ P\left(Y = \arg \max_k f_k(X) \mid \max_k f_k(X)\right) \overset{a.s.}{=} \max_k f_k(X)
\]

\[
\iff \begin{cases} \text{TCE}_p\) \((f) = 0 \\ \text{MMCE}(f) = 0 \end{cases}
\]

See Theorem 1 in [17] regarding MMCE. Note that we could not verify their claim that MMCE is a proper score, which is even contradictive to our findings. A sketch for an example where CWCE\(_p\) \((f) = 0 \iff \text{TCE}_p\) \((f) = 0\) is if \(P(Y = C \mid f_C(X)) \overset{a.s.}{=} f_C(X)\) and \(P(Y = \arg \min_k f_k(X) \mid \min_k f_k(X)) \neq \min_k f_k(X)\).

Regarding \text{TCE}_p\) \((f) = 0 \iff \text{KS}(f) = 0\):

\[
\text{TCE}_p\) \((f) = 0
\]

\[
\iff P\left(Y = \arg \max_k f_k(X) \mid \max_l f_l(X)\right) \overset{a.s.}{=} \max_m f_m(X)
\]

\[
\iff P(Y = C \mid f_C(X)) \overset{a.s.}{=} f_C(X)
\]

\[
\overset{(i)}{\implies} \int_{\sigma'} \ P(Y = C \mid f_C(X) = z) \, dp_{f_C(X)}(z) \overset{a.s.}{=} \int_{\sigma'} z \, dp_{f_C(X)}(z), \quad \forall \sigma' \subset [0, 1]
\]

\[
\iff \int_{[0, \sigma]} \ P(Y = C \mid f_C(X) = z) \, dp_{f_C(X)}(z) \overset{a.s.}{=} \int_{[0, \sigma]} z \, dp_{f_C(X)}(z), \quad \forall \sigma \in [0, 1]
\]

\[
\iff E\left[\max_{\sigma \in [0, 1]} \left| \int_{[0, \sigma]} z - P(Y = C \mid f_C(X) = z) \, dp_{f_C(X)}(z) \right| \right] = 0
\]

\[
\iff E[\text{KS}(f, C)] = 0
\]

\[
\iff \text{KS}(f) = 0
\]

(i) according to Theorem 4.22 of [12].

Regarding \text{TCE}_p\) \((f) = 0 \iff \text{ECE}(f) = 0\):

\[
\text{TCE}_p\) \((f) = 0
\]

\[
\iff P(Y = C \mid f_C(X)) \overset{a.s.}{=} f_C(X)
\]

\[
\overset{(i)}{\implies} \forall i = 1, \ldots, m: \ P(Y = C \mid f_C(X) \in B_i) \overset{a.s.}{=} E[f_C(X) \mid f_C(X) \in B_i]
\]

\[
\overset{\text{def}[2,4]}{=} \text{ECE}(f) = 0
\]

(i) with \(B_i\) defined as in definition [2,4] follows since \(P(Y = C \mid f_C(X) \in B_i) = \int_{B_i} P(Y = C \mid f_C(X) = z) \, dp_{f_C(X)}(z) \overset{a.s.}{=} \int_{B_i} f_C(X) \, dp_{f_C(X)}(z) = E[f_C(X) \mid f_C(X) \in B_i].\)

An intuition of why \text{TCE}_3\) \((f) = 0 \iff \text{ECE}(f) = 0\) is given in example 3.2 of [10].

Regarding \(2 \geq \text{BS}(f) \geq \text{CE}_2\) \((f)\):

\[
2 = ||e_1 - e_2||_2^2
\]

\[
\geq E\left[\|f(X) - e_Y\|_2^2\right]
\]

\[
\overset{\text{def}[2,4]}{=} \text{BS}(f)
\]

\[
\overset{(i)}{\geq} \text{BS}(f) - E\left[g_{BS}\left(P_{Y[f(X)]}\right)\right]
\]

\[
\overset{\text{le}[2,3]}{=} \text{CE}_{BS}(f)
\]

\[
\overset{(ii)}{=} \text{CE}_2(f)
\]
(i) $g_{BS}$ non-negative, follows from definition [2.11].
(ii) see table [1] and compare with definition [2.3].

Regarding $2 \geq CE_p(f)$:

\[
2 = \|e_1 - e_2\|_p^p \\
\geq \mathbb{E} \left[ \left\| f(X) - \mathbb{P}_{Y | f(X)} \right\|_p^p \right] \tag{12}
\]

Regarding $(CE_p(f))_+ \geq CWCE_p(f)$:

In the following, we will use Tonelli’s theorem to split the expectation into two and the Jensen’s inequality for the convex function $|\cdot|^p$.

\[
CE_p(f) = \mathbb{E} \left[ \left\| f(X) - \mathbb{P}_{Y | f(X)} \right\|_p^p \right] \\
= \sum_{k \in \mathcal{Y}} \mathbb{E} \left[ \left\| f_k(X) - \mathbb{P}(Y = k | f(X)) \right\|_p^p \right] \tag{13}
\]

Regarding $CWCE_p(f) \geq TCE_p(f)$:

We will use $F := f(X)$ for shorter notation.

\[
(CWCE_p(f))_+ \sum_{k \in \mathcal{Y}} \mathbb{E}_{f_k(X)} \left[ \left\| f_k(X) - \mathbb{P}(Y = k | f_k(X)) \right\|_p^p \right] \\
\geq \sum_{k \in \mathcal{Y}} \mathbb{E}_{f_k} \left[ \left| F_k - \mathbb{P}(Y = k | F_k) \right|_p^p \right] \\
= \sum_{k \in \mathcal{Y}} \mathbb{E}_F \left[ \left| F_k - \mathbb{P}(Y = k | F_k) \right|_p^p \right] \\
= \mathbb{E}_F \left[ \sum_{k \in \mathcal{Y}} \left| F_k - \mathbb{P}(Y = k | F_k) \right|_p^p \right] \\
\]

(i) Order all summands by $F$. We use notation of order statistics to refer to $(k)_F$ the index with the $k$th highest rank according to $F$.

(ii) From (i) follows $(1)_F = (1)_{f(X)} = \arg \max_k f_k(X) = C$.

Regarding $TCE_p(f) \geq TCE_1(f)$:
Let \( p \geq q \geq 1 \). This makes \( (\cdot)^{\frac{1}{p}} \) a convex function for positive arguments. We will show the more general \( \text{TCE}_p (f) \geq \text{TCE}_q (f) \). From this directly follows \( \text{TCE}_p (f) \geq \text{TCE}_1 (f) \).

\[
\text{TCE}_p (f) = \left( \mathbb{E} \left[ |f_C (X) - \mathbb{P} (Y = C \mid f_C (X))|^p \right] \right)^{\frac{1}{p}} \\
\geq \left( \mathbb{E} \left[ |f_C (X) - \mathbb{P} (Y = C \mid f_C (X))|^q \right] \right)^{\frac{1}{q}}
\]

(15)

Regarding \( \text{TCE}_1 (f) \geq \text{KS} (f) \):

We will show the more general \( \text{TCE}_p (f) \geq \text{KS} (f) \), from which \( \text{TCE}_1 (f) \geq \text{KS} (f) \) follows.

We will make use of the indicator function for a set \( A \) defined as \( \mathbb{1}_A (a) = \begin{cases} 1, & a \in A \\ 0, & \text{else} \end{cases} \).

\[
(\text{TCE}_p (f))^p = \mathbb{E} \left[ |f_C (X) - \mathbb{P} (Y = C \mid f_C (X))|^p \right]
\]

(16)

Regarding \( \text{TCE}_1 (f) \geq c \cdot \text{MMCE} (f) \):

This is given in the proof of Theorem 3 of [17]. Note that [17] used ECE in their theorem, but their proof is actually given for \( \text{TCE}_1 \). Since \( \text{ECE} (f) = 0 \iff \text{MMCE} (f) = 0 \), we have \( \text{ECE} (f) \geq c \cdot \text{MMCE} (f) \).

Regarding \( \text{TCE}_1 (f) \geq \text{ECE} (f) \):

A similar statement for binary models is given in Proposition 3.3 of [10] or for general models in Theorem 2 of [8]. Since our formulations differ, we provide an independent proof.

Let \( \mathcal{B} := \sigma \left( \left\{ \left\{ 0, \frac{1}{m} \right\}, \ldots, \left\{ \frac{m-1}{m}, 1 \right\} \right\} \right) \) be the \( \sigma \)-algebra generated by the binning scheme of size \( m \in \mathbb{N} \).
This is possible, since \( \parallel \) and \( \text{CWCE} \).

For all \( \parallel \) used for the ECE.

\[ T\text{CE}_1(f) = E[|f_C(X) - P(Y = C | f_C(X))|] \]
\[ = E[E[|f_C(X) - P(Y = C | f_C(X))| | \mathcal{R}] \]
\[ = \mathbb{E}[|E[f_C(X)| \mathcal{R} - P(Y = C | \mathbb{E}[f_C(X)| \mathcal{R}]|] \]
\[ = \sum_{i=1}^{m} \mathbb{P}(f(X) \in \left(\frac{i-1}{m}, \frac{i}{m}\right]) \mathbb{E}[f_C(X)| f(X) \in \left(\frac{i-1}{m}, \frac{i}{m}\right)] - \mathbb{P}(Y = C | f(X) \in \left(\frac{i-1}{m}, \frac{i}{m}\right)) \]
\[ \text{def. ECE}(f) \]
\[ \tag{17} \]

(i) We use conditional Jensen’s inequality \( \Box \).

### 9.3 Proposition 3.2

For all \( \epsilon > 0 \) and surjective \( f: \mathcal{X} \to \mathcal{P}_n \) there exists a joint distribution \( \mathbb{P}_{X,Y} \) such that for all \( E \in \{\text{MMCE}, \text{KS}, \text{ECE}, \text{TCE}_p, \text{CWCE}_p | 1 \leq p \in \mathbb{R}\} : \)

\[ E(f) = 0 \land \text{CE}_2(f) \geq 1 - \frac{1}{n} - \epsilon. \]

**Proof.** Assume arbitrary \( \epsilon > 0 \) and surjective \( f: \mathcal{X} \to \mathcal{P}_n \). Choose \( \mathbb{P}_{X,Y} \) such that \( E[|f(X)|^2] \leq \frac{1}{n} + \epsilon \) and

\[ \mathbb{P}(Y = k | f(X)) = \begin{cases} 1 & \text{, with probability } f_k(X) \\ 0 & \text{, else.} \end{cases} \]

This is possible, since \( |.|^2: \mathcal{P}_n \to [\frac{1}{n}, 1] \) and \( f \) are surjective, from which follows \( \forall \epsilon > 0 \exists x \in \mathcal{X}: \; \frac{1}{n} + \epsilon \geq \|f(x)\|^2. \)

Write \( F := f(X) \) and \( Y := e_Y \) (one-hot encoded \( Y \)).

Then we have \( \mathbb{P}(Y = k | F_k) = \mathbb{E}[Y_k | F_k] = \mathbb{E}_{F_k} \mathbb{E}[Y_k | F] F_k = F_k \) and consequently \( \text{CWCE}_p(f) = 0. \) The other errors follow from Theorem 3.1. But we also have

\[ \text{CE}_2(f) = E[|P_{Y|f(X)} - f(X)|^2] \]
\[ = E[|E[Y | F] - F|^2] \]
\[ = \sum_{k \in \mathcal{Y}} E[(E[Y_k | F] - F_k)^2] \]
\[ = \sum_{k \in \mathcal{Y}} E[(E[Y_k | F])^2] - 2E[E[Y_k | F]F_k] + E[F_k^2] \]
\[ = \sum_{k \in \mathcal{Y}} E[E[Y_k | F]] - 2E[E[Y_k | F]F_k] + E[F_k^2] \]
\[ = 1 - 2 \sum_{k \in \mathcal{Y}} E[E[Y_k | F]F_k] + \sum_{k \in \mathcal{Y}} E[F_k^2] \]
\[ = 1 - 2 \sum_{k \in \mathcal{Y}} E[E[Y_k | F_k]F_k] + \sum_{k \in \mathcal{Y}} E[F_k^2] \]
\[ = 1 - 2 \sum_{k \in \mathcal{Y}} E[F_k^2] + \sum_{k \in \mathcal{Y}} E[F_k^2] \]
\[ = 1 - \sum_{k \in \mathcal{Y}} E[F_k^2] \]
\[ = 1 - \mathbb{E}||F||^2 \]
\[ \geq 1 - \frac{1}{n} - \epsilon \]

17
9.4 Proposition 3.3

Define $t^f : \mathcal{P}_n \to \mathcal{P}_n$ to replace the largest entry in its input with the accuracy of model $f$. The other entries are set such that the output is a unit vector.

For all models $f : \mathcal{X} \to \mathcal{P}_n$ and $E \in \{MMCE, KS, ECE, TCE_p \mid 1 \leq p \in \mathbb{R}\}$ we have

$$E (t^f \circ f) = 0 \quad \land \quad \text{ACC} (t^f \circ f) = \text{ACC} (f).$$

But, in general $\text{CE}_p \left( t^f \circ f \right) > 0$.

Proof. Formal definition of $t^f$ is located in Appendix 10.1 and proof follows from combination of Proposition 9.2 and Theorem 3.1.

9.5 Lemma 4.1

Let $\mathcal{D}$ be a set of arbitrary distributions for which exists a proper score $S$. Assume we have random variables $Q$ and $Y$ with $Q, P_Y, P_{Y|Q} \in \mathcal{D}$ for which $g_S (P_Y), \mathbb{E} \left[ g_S (P_{Y|Q}) \right], \mathbb{E} \left[ \|S (Q, Y)\| \right], \mathbb{E} \left[ \|S (P_Y, Y)\| \right] < \infty$. The last two expectations are required for Fubini’s theorem.

$$\mathbb{E} \left[ S (Q, Y) \right] = \int \int S (q, y) \, dP_{Y|Q} (y, q)$$

\[ \begin{aligned}
&= \int \int S (q, y) \, dP_{Y|Q=q} (y) \, dP_Q (q) \\
&= \int s_S (q, P_{Y|Q=q}) \, dP_Q (q) \\
&= \mathbb{E} \left[ s_S (Q, P_{Y|Q}) \right] + \mathbb{E} \left[ s_S (P_Y, P_{Y|Q}) \right] - \mathbb{E} \left[ s_S (P_{Y|Q}, P_{Y|Q}) \right] \\
&= s_S (P_Y, P_Y) - s_S (P_Y, P_Y) + \mathbb{E} \left[ s_S (P_{Y|Q}, P_{Y|Q}) \right] + \mathbb{E} \left[ d_S (Q, P_{Y|Q}) \right] \\
&= s_S (P_Y, P_Y) - S (P_Y, y) \, dP_Y (y) + \mathbb{E} \left[ s_S (P_{Y|Q}, P_{Y|Q}) \right] + \mathbb{E} \left[ d_S (Q, P_{Y|Q}) \right] \\
&= s_S (P_Y, P_Y) - \int S (P_Y, y) \, dP_Y (y) + \mathbb{E} \left[ s_S (P_{Y|Q}, P_{Y|Q}) \right] + \mathbb{E} \left[ d_S (Q, P_{Y|Q}) \right] \\
&= s_S (P_Y, P_Y) - \int S (P_Y, y) \, dP_{Y|Q=q} (y) \, dP_Q (q) + \mathbb{E} \left[ s_S (P_{Y|Q}, P_{Y|Q}) \right] + \mathbb{E} \left[ d_S (Q, P_{Y|Q}) \right] \\
&= s_S (P_Y, P_Y) - \mathbb{E} \left[ s_S (P_{Y|Q}, P_{Y|Q}) \right] + \mathbb{E} \left[ d_S (Q, P_{Y|Q}) \right].
\end{aligned} \]

9.6 Theorem 4.3

For all proper calibration errors with $\inf_{P \in \mathcal{D}} g_S (P) \in \mathbb{R}$, there exists an associated calibration upper bound

$$\mathcal{B}_S (f) \geq \text{CE}_S (f)$$

defined as $\mathcal{B}_S (f) := \mathbb{E} \left[ S (f (X), Y) \right] - \inf_{P \in \mathcal{D}} g_S (P)$. Under a classification setting and further mild conditions, it is asymptotically equal to the $\text{CE}_S$ with increasing model accuracy, i.e.

$$\lim_{\text{ACC}(f) \to 1} \mathcal{B}_S (f) - \text{CE}_S (f) = 0.$$
Proof. Regarding existence of upper bound
Assuming $\inf_{Q \in \mathcal{P}} g_S(Q) \in \mathbb{R}$.

\[
CE_S(f) \leq \mathbb{E}[S(f(X), Y)] - \mathbb{E}[\mathbb{E}[S(Y|f(X))]] - \mathbb{E}[S(f(X), Y)] - \mathbb{E}[\inf_{Q \in \mathcal{P}} g_S(Q)] = \mathbb{E}[S(f(X), Y)] - \inf_{Q \in \mathcal{P}} g_S(Q)
\]

th. (iii) Since (ii) follows from initial condition.

Regarding accuracy limes
Assuming mild conditions $g_S: \mathcal{P} \rightarrow \mathbb{R}$ is continuous and $g_S(e_1) = g_S(e_2) = \cdots = g_S(e_n)$. See Figure 2 in [35] for an example when this is violated. $S$ does not have to be symmetric for this to hold.

\[
\lim_{\text{ACC}(f) \rightarrow 1} CE_S(f) - \mathcal{U}_S(f)
\]

\[
\lim_{\text{ACC}(f) \rightarrow 1} CE_S(f) - \mathbb{E}[S(f(X), Y)] + \inf_{Q \in \mathcal{P}} g_S(Q)
\]

\[
\lim_{\text{ACC}(f) \rightarrow 1} \mathbb{E}[S(f(X), Y)] - \mathbb{E}[\mathbb{E}[S(Y|f(X))]] - \mathbb{E}[S(f(X), Y)] + \inf_{Q \in \mathcal{P}} g_S(Q)
\]

\[
\lim_{\text{ACC}(f) \rightarrow 1} \mathbb{E}[S(f(X), Y)] - \mathbb{E}[\mathbb{E}[S(Y|f(X))]] + \inf_{Q \in \mathcal{P}} g_S(Q)
\]

\[
\lim_{\text{ACC}(f) \rightarrow 1} \mathbb{E}[S(f(X), Y)] - \mathbb{E}[\mathbb{E}[S(Y|f(X))]] + \inf_{Q \in \mathcal{P}} g_S(Q)
\]

\[
\lim_{\text{ACC}(f) \rightarrow 1} \mathbb{E}[S(f(X), Y)] - \mathbb{E}[\mathbb{E}[S(Y|f(X))]] + \inf_{Q \in \mathcal{P}} g_S(Q)
\]

\[
\lim_{\text{ACC}(f) \rightarrow 1} \mathbb{E}[S(f(X), Y)] - \mathbb{E}[\mathbb{E}[S(Y|f(X))]] + \inf_{Q \in \mathcal{P}} g_S(Q)
\]

(i) Perfect accuracy results in deterministic predictions, i.e. $\forall z \in \mathcal{P}_n: \lim_{\text{ACC}(f) \rightarrow 1} \mathbb{E}[S(f(X), Y)] = z \in \{e_i \mid n \geq i \in \mathbb{N}\}$. If we define $i: \mathcal{P} \rightarrow \mathbb{N}$ as $i(X) := \arg\max_{k} \lim_{\text{ACC}(f) \rightarrow 1} \mathbb{P}(Y = k | f(X))$, then we have $e_{i(X)} = \lim_{\text{ACC}(f) \rightarrow 1} \mathbb{E}[S(f(X))]$.

(ii) Follows from initial condition.

(iii) Since $g_S$ is concave and by the definition of $\mathcal{P}_n$, we have

\[
\forall z \in \mathcal{P}_n \exists \lambda_1, \ldots, \lambda_n \geq 0, \sum_k \lambda_k = 1: g_S(z) = g_S \left( \sum_k \lambda_k e_k \right) \geq \sum_k \lambda_k g_S(e_k) = \sum_k \lambda_k g_S(e_1) = g_S(e_1).
\]

From this follows that $g_S(e_1) = \inf_{Q \in \mathcal{P}_n} g_S(Q)$.

\[\square\]

9.7 Proposition 4.4

Given injective functions $h, h': \mathcal{P} \rightarrow \mathcal{P}$ we have

\[
\mathcal{U}_S(h \circ f) - \mathcal{U}_S(f) = CE_S(h \circ f) - CE_S(f)
\]

\[
\mathcal{U}_S(h \circ f) > \mathcal{U}_S(h' \circ f) \iff CE_S(h \circ f) > CE_S(h' \circ f)
\]

and (assuming $S$ is differentiable)

\[
\frac{d\mathcal{U}_S(h \circ f)}{dh} = \frac{dCE_S(h \circ f)}{dh}
\]
Proof.

$$\mathcal{W}_S (h \circ f) - \mathcal{W}_S (h' \circ f)$$

th \(\begin{array}{l}
\text{theorem} \\
\inf_{Q \in \mathcal{P}_n} \mathbb{E} [S (h \circ f (X), Y)] - \inf_{Q \in \mathcal{P}_n} g_S (Q) \\
= \mathbb{E} [S (h \circ f (X), Y)] - \mathbb{E} [S (h' \circ f (X), Y)] \\
= \mathbb{E} [S (h \circ f (X), Y)] - \mathbb{E} [g_S (P_{Y|f(X)})] + \mathbb{E} [g_S (P_{Y|f(X)})] \\
\end{array} \)

(22)

(23)

(i) Since \(h\) is injective, we have \(\forall z \in \mathcal{P}_n\): \(\{ x \in X | f (x) = z \} = \{ x \in X | h \circ f (x) = h (z) \}\) and \(\{ (x, y) \in X \times \mathcal{Y} | f (x) = z \} = \{ (x, y) \in X \times \mathcal{Y} | h \circ f (x) = h (z) \}\). Consequently \(P (Y | f (X) = z) = \frac{P (y | f (X) = z)}{\sum_{i \in \mathcal{Y}} P (y | f (X) = z)} = P (Y | h \circ f (X) = h (z))\).

\[ \square \]

10 Recalibration transformations

We provide several recalibrations which map to a finite set and are accuracy preserving and calibrated in some sense. They all have unbiased estimators.

10.1 Zero TCE and accuracy-preserving, but not strongly calibrated

Assume we are given model \(f: X \rightarrow \mathcal{P}_n\).

Define \(\sigma: \mathcal{P}_n \times \mathcal{P}_n \rightarrow \mathcal{P}_n\) order the entries of its second input according to the values given in the first input. Let \(\sigma^{-1}: \mathcal{P}_n \times \mathcal{P}_n \rightarrow \mathcal{P}_n\) revert the ordering in the second input according to the entries of its first input. For easier notation, we will write \(\sigma_u (v) := \sigma (u, v)\) and \(\sigma^{-1}_u (v) := \sigma^{-1} (u, v)\), which gives \(\forall u, v \in \mathcal{P}_n\): \(\sigma^{-1}_u \circ \sigma_u (v) = v\). I.e. \(\sigma^{-1}_u\) is the inverse of \(\sigma_u\) given \(u\).

We will require the following.

Lemma 10.1. \(\forall u, v \in \mathcal{P}_n\): \(\arg \max_{k} (\sigma^{-1}_u \circ \sigma_u (v))_k = \arg \max_{k} u_k\)

Proof. Assume \(u, v \in \mathcal{P}_n\) arbitrary. We have \(\forall k\): \((\sigma_u (v))_k \geq (\sigma_v (v))_k \land (\sigma_u (u))_k \geq (\sigma_v (u))_k\). Consequently, \(\arg \max_k (\sigma^{-1}_u \circ \sigma_u (v))_k = \arg \max_k (\sigma^{-1}_u \circ \sigma_u (u))_k = \arg \max_k u_k\).

Define \(c_f := (\text{ACC}(f), \frac{1}{n-1} \text{ACC}(f), \ldots, \frac{1}{n-1} \text{ACC}(f))^{\top} \in \mathcal{P}_n\).

Proposition 10.2. The function \(t^f : \mathcal{P}_n \rightarrow \mathcal{P}_n\) defined as \(t^f (p) := \sigma^{-1}_p (c_f)\) transforms \(f\) such that \(\text{TCE}_{\mathcal{B}} (t^f \circ f) = 0\) and \(\text{ACC}(t^f \circ f) = \text{ACC}(f)\).

Proof. Regarding accuracy:
Since we can in every practical setting assume \(\text{ACC}(f) > \frac{1}{n-1} \text{ACC}(f)\) and by Lemma 10.1 we have \(\arg \max_k t^f_k (f (X)) = \arg \max_k f_k (X)\), since \(c_f\) is ordered. This states that \(t^f\) is accuracy-preserving.
Regarding zero TCE:
Note that $\text{ACC}(f) = \mathbb{P}(Y = \arg \max_k f_k(X))$. Using this, we have
$$\mathbb{P}(Y = \arg \max_k t_k^f \circ f(X) \mid \max_k t_k^f \circ f(X)) = \mathbb{P}(Y = \arg \max_k f_k(X) \mid \text{ACC}(f)) = \mathbb{P}(Y = \arg \max_k f_k(X)) = \text{ACC}(f) = \max_k t_k^f \circ f(X)$. It follows $\text{TCE}_p(t^f \circ f) = 0$. □

$\text{CE}_p(t^f \circ f) > 0$, since in general $\mathbb{P}(Y = \arg \max_k F_k \mid \max_k F_k) = \max_k F_k$ does not imply $\mathbb{P}(Y = k \mid F) = F_k$ for random variables $F$ and $Y$, which is required for the error to be zero [S].

10.2 Strongly calibrated and accuracy-preserving

The binary case is directly given in the multi-class case, but if we only have a scalar output, which is feasible for higher number of classes.

Let

10.2.1 Binary case (scalar output)

Assume we are given $f: \mathcal{X} \rightarrow [0, 1]$. 

Define $t^f: [0, 1] \rightarrow [0, 1]$ as

$$t^f(p) = \begin{cases} 
  \mathbb{P}(Y = 1 \mid f(X) < 0.5) & \text{if } p < 0.5 \\
  \mathbb{P}(Y = 1 \mid f(X) \geq 0.5) & \text{else}
\end{cases} \quad (24)
$$

The first line has as unbiased estimator the precision (or positive predictive value), the second the false omission rate.

This gives

$$\mathbb{P}(Y = 1 \mid t^f \circ f(X)) = \begin{cases} 
  \mathbb{P}(Y = 1 \mid \mathbb{P}(Y = 1 \mid f(X) < 0.5)) & \text{if } f(X) < 0.5 \\
  \mathbb{P}(Y = 1 \mid \mathbb{P}(Y = 1 \mid f(X) \geq 0.5)) & \text{else}
\end{cases} \quad (25)
$$

$$= \begin{cases} 
  \mathbb{P}(Y = 1 \mid f(X) < 0.5) & \text{if } f(X) < 0.5 \\
  \mathbb{P}(Y = 1 \mid f(X) \geq 0.5) & \text{else}
\end{cases} \quad (25)
$$

i.e. $t^f \circ f$ is strongly calibrated. Further, if $\mathbb{P}(Y = 1 \mid f(X) < 0.5) < \mathbb{P}(Y = 1 \mid f(X) \geq 0.5)$, then $t^f \circ f$ has the same accuracy as $f$. This can be assumed as given for any meaningful classifier. The reduction in sharpness directly follows from the analog proof in the multi-class case.

10.2.2 Multi-class case (vector output)

Let $r: \mathcal{P}_n \rightarrow A$ with $A = \left\{a \in \{0, 1\}^K \mid \sum_k a_k = 1 \right\}$ be defined as $r(p) := e_{\arg \max_k p_k}$. In words, $r$ returns a vector of only zeros except a ’1’ at index $\arg \max_k p_k$ for input $p \in \mathcal{P}_n$.

Define $t^f: \mathcal{P}_n \rightarrow \mathcal{P}_n$ as

$$t^f(p) = \mathbb{P}(Y \mid r \circ f(X) = r(p)) \quad (26)
$$

(For easier notation, we say $\mathbb{P}(Y) \in \mathcal{P}_n$.)

Given a dataset $\{(X_1, Y_1), \ldots, (X_m, Y_m)\}$, an unbiased estimator of $\mathbb{P}(Y \mid r \circ f(X) = a) \forall a \in A$ is

$$P_n = \frac{1}{|n|} \sum_{i \in I_n} e_{Y_i} \quad \text{with } I_n = \{i \in \{1, \ldots, m\} \mid r \circ f(X_i) = a\}$. And since $|A| = n$, estimation is also feasible for higher number of classes.
We also have

\[
\mathbb{P}(Y | t^f \circ f(X)) = \mathbb{P}(Y | \mathbb{P}(Y | r \circ f(X) = r \circ f(X))) \\
= \mathbb{P}(Y | \mathbb{P}(Y | r \circ f(X))) \\
= \mathbb{P}(Y | r \circ f(X)) \\
= t^f \circ f(X)
\]  

(27)

Consequently, \( t^f \circ f \) is strongly calibrated.

If \( \arg \max_k f_k(X) = \arg \max_k \mathbb{P}(Y = k | \arg \max_k f_k(X)) \), then \( \arg \max_k f_k(X) = \arg \max_k \mathbb{P}(Y = k | r \circ f(X)) = \arg \max_k \mathbb{P}(Y = k | r \circ f(X) = r \circ f(X)) = \arg \max_k t^f \circ f(X) \), i.e. \( t^f \) is accuracy preserving. Recall that \( \arg \max_k f_k(X) \) is the predicted top-label, making \( \arg \max_k \mathbb{P}(Y = k | \arg \max_k f_k(X)) \) the most likely outcome given a predicted top-label. So, we can restate the above as: \( t^f \) is accuracy preserving if for every predicted top-label the most likely outcome is that label. This should hold in every meaningful practical setting, or else \( t^f \) might as well improve the accuracy.

\( t^f \circ f \) has lower sharpness as \( f \) w.r.t. a proper score \( S \). This is a special case of the following proposition, where we write \( \text{SHARP}_S(f) \) as the sharpness of model \( f \) given by the sharpness term in Lemma 4.1 of a proper score \( S \).

**Proposition 10.4.** Assume Lemma 4.1 holds given a proper score \( S \). For a function \( m: \mathcal{P}_n \to \mathcal{P}_n \) and model \( f: \mathcal{X} \to \mathcal{P}_n \), we have

\[
\text{SHARP}_S(f) \geq \text{SHARP}_S(m \circ f). 
\]

**Proof.** Since we assumed Lemma 4.1 holds, the conditions for Fubini’s theorem are met. We will use:

\[
\text{SHARP}_S(f)
\]

\[
\text{def} \quad \text{Lebesgue differentiation} \quad E \left[ d_S \left( \mathbb{P}_Y, \mathbb{P}_{Y|f(X)} \right) \right]
\]

\[
\text{def} \quad \text{definition} \quad E \left[ s_S \left( \mathbb{P}_Y, \mathbb{P}_{Y|f(X)} \right) \right] - E \left[ g_S \left( \mathbb{P}_{Y|f(X)} \right) \right]
\]

\[
= \int S(\mathbb{P}_Y, y) d\mathbb{P}_{Y|f(X)}(y) = E \left[ g_S \left( \mathbb{P}_{Y|f(X)} \right) \right]
\]

\[
\text{Fubini} \quad E \left[ g_S \left( \mathbb{P}_Y \right) - E \left[ g_S \left( \mathbb{P}_{Y|f(X)} \right) \right] \right]
\]

Now, we can show

\[
\text{SHARP}_S(f)
\]

\[
\text{eq} \quad g_S \left( \mathbb{P}_Y \right) - E \left[ g_S \left( \mathbb{P}_{Y|f(X)} \right) \right] \geq g_S \left( \mathbb{P}_Y \right) - E_{m \circ f(X)} \left[ E_{f(X)} \left[ g_S \left( \mathbb{P}_{Y|f(X)} \right) \right] \right]
\]

\[
\text{Jensen} \quad g_S \left( \mathbb{P}_Y \right) - E_{m \circ f(X)} \left[ g_S \left( E_{f(X)} \left( \mathbb{P}_{Y|f(X)} \right) \right) \right] \geq g_S \left( \mathbb{P}_Y \right) - E_{m \circ f(X)} \left[ g_S \left( E_{f(X)} \left( \mathbb{P}_{Y|f(X)} \right) \right) \right]
\]

\[
\text{eq} \quad \text{SHARP}_S(m \circ f)
\]
If the underlying score is the log score, then the sharpness is the mutual information between predictions and target random variable. Consequently, we can interpret the sharpness as generalized mutual information. This gives the proposition the following intuitive meaning: There exists no function, that can transform a random variable in a way such that the mutual information with another random variable is increased. Or, in other words, we cannot add ‘information’ to a random variable by transforming it in a deterministic way.

11 Proper U-scores

In this section we introduce a generalization of proper scores. Based on U-statistics, we define proper U-scores. This allows us to naturally extend the definition of proper calibration errors to be based on proper U-scores instead of just proper scores. Consequently, we can cover more calibration errors with desired properties. For example, we can show that the squared KCE \[21\] is a proper calibration error based on a U-score (but not on a conventional score). The squared KCE has an unbiased estimator, thus, this extension of the definition of proper calibration errors has substantial practical value.

11.1 Background

Let \(X_1, \ldots, X_n\) be \(n\) iid random variables and \(\phi(x_1, \ldots, x_r)\) a function with \(r \leq n\). Let \(P = \{a \in \{1, \ldots, n\}^r \mid a_1 < \cdots < a_r\}\) be the set of \(r\) sized ordered permutations out of \(n\), i.e. \(|P| = \binom{n}{r}\). Then
\[
U = \frac{1}{|P|} \sum_{a \in P} \phi(X_{a_1}, \ldots, X_{a_r})
\]
is a unbiased minimum-variance estimator (UMVE) of \(E[\phi(X_1, \ldots, X_r)]\) and called U-statistic \[43\].

11.2 Contributions

Assume we have two measure spaces \((\mathcal{X}, \mathcal{F}_X)\) and \((\mathcal{Y}, \mathcal{F}_Y)\), and corresponding \(\mathcal{P}_X\) and \(\mathcal{P}_Y\) sets of possible probability measures. We want to score a conditional distribution \(P: \mathcal{X} \rightarrow \mathcal{P}_Y\) given another conditional distribution \(Q: \mathcal{X} \rightarrow \mathcal{P}_Y\).

Definition 11.1. A U-scoring rule \(S\) is a function of the form
\[
S : \mathcal{P}_Y^r \times \mathcal{Y}^r \rightarrow \mathbb{R}
\]
with \(r \in \mathbb{N}\) and \(\overline{\mathbb{R}} := \mathbb{R} \cup \{-\infty, \infty\}\).

It takes \(r\) predictions and events and returns a score. For \(r = 1\), U-scoring rules are scoring rules in the common definition.

Definition 11.2. A U-scoring function \(s_S\) based on a U-scoring rule \(S\) is defined as
\[
s_S : \mathcal{P}_Y^r \rightarrow \overline{\mathbb{R}}
\]
\[
(P_1, \ldots, P_r, Q_1, \ldots, Q_r) \rightarrow \int_{\mathcal{Y}^r} S(P_1, \ldots, P_r, y_1, \ldots, y_r) \, d(Q_1 \times \cdots \times Q_r)(y)
\]
(30)

For \(r = 1\), U-scoring functions are scoring functions in the common definition. If \(Q_1, \ldots, Q_r\) are the distributions of \(Y_1, \ldots, Y_r\) we can also write \(s(P_1, \ldots, P_r, Q_1, \ldots, Q_r) = \mathbb{E}[S(P_1, \ldots, P_r, Y_1, \ldots, Y_r)]\).

Definition 11.3. A U-scoring function \(s_S\) (and its U-scoring rule \(S\)) is defined to be proper if and only if
\[
\forall P \in \mathcal{P}_X, \ X_1, \ldots, X_r \overset{iid}{\sim} P, \ \forall P, Q: \mathcal{X} \rightarrow \mathcal{P}_Y:
\]
\[
\mathbb{E}S_S(P(X_1), \ldots, P(X_r), Q(X_1), \ldots, Q(X_r)) \geq \mathbb{E}S_S(Q(X_1), \ldots, Q(X_r), Q(X_1), \ldots, Q(X_r))
\]
(31)

and strictly proper if and only if additionally
\[
\forall P \in \mathcal{P}_X, \ X_1, \ldots, X_r \overset{iid}{\sim} P, \ \forall P, Q: \mathcal{X} \rightarrow \mathcal{P}_Y:
\]
\[
Q \neq P \implies \mathbb{E}S_S(P(X_1), \ldots, P(X_r), Q(X_1), \ldots, Q(X_r)) > \mathbb{E}S_S(Q(P_1), \ldots, Q(P_r), Q(P_1), \ldots, Q(P_r))
\]
(32)
In words, $s_g$ (or $S$) is proper if comparing $Q$ with itself gives the best expected value, and strictly proper if no other $P \neq Q$ can achieve this value. The U-statistic of a proper $s_g$ is a UMVE [43]. For $r = 1$, proper U-scores are identical to proper scores if $\mathcal{P}_X$ is sufficiently large. This holds since for function $f: \mathcal{X} \rightarrow \mathbb{R}$ and appropriate $\mathcal{P}_X$ we have: $(\forall \mu \in \mathcal{P}_X: \int f d\mu = 0) \iff f = 0$.

**Definition 11.4.** $g(Q_1, \ldots, Q_r) = s(Q_1, \ldots, Q_r, Q_1, \ldots, Q_r)$ is called the (generalized or associated) entropy.

**Definition 11.5.** Given a proper U-score $S$, the associated U-divergence $d$ is defined as

$$d_S : \mathcal{P}_Y^r \rightarrow \mathbb{R}_{\geq 0}$$

$$(P_1, \ldots, P_r, Q_1, \ldots, Q_r) \mapsto s_S(P_1, \ldots, P_r, Q_1, \ldots, Q_r) - g_S(Q_1, \ldots, Q_r).$$

If $S$ is a strictly proper U-score, $Q_1, \ldots, Q_r$ iid and $P_1, \ldots, P_r$ iid, then $\mathbb{E}d_S$ is zero if and only if $\forall i \in \{1, \ldots, r\}$ : $Q_i \overset{d}{=} P_i$. This follows directly by setting $P_i = P(X_i)$ and $Q_i = Q(X_i)$ in equation [32].

Assuming $P_1, \ldots, P_r$ are random variables and $\mathbb{P}_{Y|P_1}, \ldots, \mathbb{P}_{Y|P_r} \in \mathcal{P}_Y$ are the conditional distribution of independent random variables $Y_1, \ldots, Y_r \sim \mathbb{P}_Y$, where each $Y_i$ only depends on $P_i$. Under the condition that $g_S(\mathbb{P}_Y, \ldots, \mathbb{P}_Y), \mathbb{E}[g_S(\mathbb{P}_{Y|P_1}, \ldots, \mathbb{P}_{Y|P_r})], \mathbb{E}[\{S(P_1, \ldots, P_r, Y_1, \ldots, Y_r)\}], \mathbb{E}[\{S(\mathbb{P}_Y, \ldots, \mathbb{P}_Y, Y_1, \ldots, Y_r)\}] < \infty$, we have the decomposition

$$\mathbb{E}[S(P_1, \ldots, P_r, Y_1, \ldots, Y_r)]$$

$$= \mathbb{E}[s_S(P_1, \ldots, P_r, \mathbb{P}_{Y|P_1}, \ldots, \mathbb{P}_{Y|P_r})]$$

$$= g_S(\mathbb{P}_Y, \ldots, \mathbb{P}_Y)$$

$$+ \mathbb{E}[d_S(P_1, \ldots, P_r, \mathbb{P}_{Y|P_1}, \ldots, \mathbb{P}_{Y|P_r})]$$

$$- \mathbb{E}[d_S(\mathbb{P}_Y, \ldots, \mathbb{P}_Y, \mathbb{P}_{Y|P_1}, \ldots, \mathbb{P}_{Y|P_r})].$$

Proof is identical to proof of Lemma [4.1]. The first term is the generalized entropy, the second the calibration, and the third the sharpness term.

Thus, every proper U-score $S$ induces a proper calibration error defined as

$$\text{CE}_S(f)$$

$$= \mathbb{E}[d_S(f(X_1), \ldots, f(X_r), \mathbb{P}_{Y|f(X_1)}, \ldots, \mathbb{P}_{Y|f(X_r)})]$$

with iid $X_1, \ldots, X_r$.

Since proper U-scores are identical to proper scores for $r = 1$, this definition of proper calibration errors does not contradict definitions or findings in the main paper. For any strictly proper U-score $S$, $\text{CE}_S$ of model $f$ is zero if and only if $f$ is strongly calibrated. This directly follows from the property of the U-divergence. But, it should be noted that we cannot assume every property holding for $r = 1$ also holds for $r \in \mathbb{N}$. Investigating this can be seen as potential future work.

An example with $r = 2$: For positive definite kernel matrix $k$, define

$$S(P_1, P_2, y_1, y_2) := (P_1 - e_{y_1})^T k(P_1, P_2) (P_2 - e_{y_2})$$

which gives

$$g_S(Q_1, Q_2) = 0$$

and

$$d_S(P_1, P_2, Q_1, Q_2) = (P_1 - Q_1)^T k(P_1, P_2) (P_2 - Q_2)$$
and the calibration term

\[
E \left[ d_S \left( P_1, P_2, \mathbb{P}_{Y|P_1}, \mathbb{P}_{Y|P_2} \right) \right] \\
= E \left[ \left( P_1 - \mathbb{P}_{Y|P_1} \right)^\top k \left( P_1, P_2 \right) \left( P_2 - \mathbb{P}_{Y|P_2} \right) \right] 
\]

(39)

If \( P_1, P_2 \sim \mathbb{P}_{f(X)} \), then this is the squared KCE (SKCE) of \( f \) [21]. \( S \) being proper follows from proves in [21]. They show SKCE uniquely identifies if \( f(X) = \mathbb{P}_{Y|f(X)} \) for arbitrary \( f(X) \) and \( \mathbb{P}_{Y|f(X)} \), consequently the expectation of \( d_S \) is only zero under the same condition, from which follows that \( S \) is strictly proper. Indeed, to the author’s best knowledge, the SKCE is the first proper calibration error with an unbiased estimator.

12 Extended experiments

In this section, we provide further details of the experimental setup and report additional results. This includes results in the squared space, where the upper bound estimator is minimum-variance unbiased.

12.1 Details on experimental setup

The experiments are conducted across several model-dataset combinations, for which logit sets are openly accessible [3][26][13]. This includes the models LeNet 5 [44], ResNet 50 (with and without pretraining), ResNet 50 NTS, ResNet 101 (with and without pretraining) ResNet 110, ResNet 110 SD, ResNet 152, ResNet 152 SD [45], Wide ResNet 32 [38], DenseNet 40, DenseNet 161 [39], and PNASNet5 Large [46] and the datasets CIFAR10, CIFAR100 [40], and ImageNet [41]. We did not conduct model training by ourselves, and refer to [26] and [13] for further details. Validation and test set splits are predefined in every logit set. We include TS, ETS, and DIAG as injective recalibration methods. For optimization of TS and ETS, we modified the available implementation of [12] and used the validation set as calibration set. For DIAG, we used the exact implementation of [13].

For every dataset we investigate ten ticks of different (sampled) test set sizes. The ticks are determined to be equally apart in the log₂ space. The minimum is always 100 and the maximum the full available test set size. We use repeated sampling with subsequent averaging to counteract the increased estimation variance for low test set sizes. The estimated standard errors are also shown in the plots, but they are often barely visible. The number of samples in each tick is along the following:

- Tick 1 (\( n = 100 \)): 20000
- Tick 2: 15842
- Tick 3: 12168
- Tick 4: 8978
- Tick 5: 6272
- Tick 6: 4050
- Tick 7: 2312
- Tick 8: 1058
- Tick 9: 288
- Tick 10 (full test set): 2

The seeds for the sampling of the experiments have been saved. Since we choose the amount of samples such that the estimation standard error is low, we expect similar results no matter the chosen seed. All experiments have been computed on a machine with 1007 GB RAM and two Intel(R) Xeon(R) Gold 6230R CPU @ 2.10GHz.

3https://github.com/markus93/NN_calibration/ and https://github.com/AmirooR/IntraOrderPreservingCalibration
12.2 Estimated model calibration

Calibration errors according to different estimators and for different model-dataset combinations are shown in figure 4 and first row of figure 6 (in squared space). These experiments confirm that the proposed upper bound is stable across a multitude of settings.

12.3 Recalibration improvement

In the main text we investigated recalibration improvement of common estimators for the calibration error and compared their reliability to RBS. According to Proposition 4.4 and since RBS is asymptotically unbiased and consistent, it can be regarded as a reliable approximation of the real improvement of the recalibration methods. However, if we move to the squared space, our proposed upper bound is even provably reliable since it has a minimum-variance unbiased estimator. This motivates further experiments comparing existing calibration errors in the squared space, which we describe in the following. Here, we first report additional results comparing common estimators to RBS; we then report results in the squared space. We start with a formal description of the problem and experimental setup.

Let $D$ be a sampled subset of the full test set. Let $f$ be the underlying model and $h$ an optimized recalibration method. Let $e$ be an calibration error estimator taking a dataset and a model as inputs. The recalibration improvement according to estimator $e$ is estimated via $e(D,f) - e(D,h \circ f)$.

Recalibration improvement of common estimators We compute the recalibration improvement of common estimators on several test set samples of a given size and plot the average of these on the y-axis. We extend the results reported in the main text by covering additional datasets, models and architectures. These extended experiments confirm the findings reported in the main text, namely that only RBS reliably quantifies the improvement in calibration error after recalibration (Fig. 5; standard errors are shown).

Recalibration improvement in the squared space The recalibration improvement in the squared space according to estimator $e$ is estimated via $(e(D,f))^2 - (e(D,h \circ f))^2$. Only our proposed upper bound yields provably unbiased estimates of the true recalibration improvement w.r.t. CE$_2$. In contrast to our approach, all other estimators are sensitive to test set size and/or substantially misestimate the true recalibration improvement in squared space (figure 6).
Figure 4: Different calibration error estimates versus the test set size. The red line corresponds to the square root of the Brier score which is an upper bound of the true $\sqrt{CE_2}$. The other estimators are lower bounds.
Figure 5: Different calibration improvement estimates versus the test set size. The red line corresponds to the square root of the Brier score.
Figure 6: **First row:** Different squared calibration error estimates versus the test set size. The red line corresponds to the Brier score which is an upper bound of the true CE$_2$. The other errors are lower bounds. **Second row:** Estimated improvements in the squared space of injective recalibration methods in different settings. Our approach captures the true improvement w.r.t. CE$_2$ in an unbiased manner.