On the Usefulness of the Fit-on-the-Test View on Evaluating Calibration of Classifiers

Markus Kängsepp\textsuperscript{1,*}, Kaspar Valk\textsuperscript{1} and Meelis Kull\textsuperscript{1}

\textsuperscript{1}*Institute of Computer Science, University of Tartu, Narva mnt, Tartu, 51009, Tartumaa, Estonia.

*Corresponding author(s). E-mail(s): markus.kangsepp@ut.ee; Contributing authors: kaspar.valk@ut.ee; meelis.kull@ut.ee;

Abstract

Every uncalibrated classifier has a corresponding true calibration map that calibrates its confidence. Deviations of this idealistic map from the identity map reveal miscalibration. Such calibration errors can be reduced with many post-hoc calibration methods which fit some family of calibration maps on a validation dataset. In contrast, evaluation of calibration with the expected calibration error (ECE) on the test set does not explicitly involve fitting. However, as we demonstrate, ECE can still be viewed as if fitting a family of functions on the test data. This motivates the fit-on-the-test view on evaluation: first, approximate a calibration map on the test data, and second, quantify its distance from the identity. Exploiting this view allows us to unlock missed opportunities: (1) use the plethora of post-hoc calibration methods for evaluating calibration; (2) tune the number of bins in ECE with cross-validation. Furthermore, we introduce: (3) benchmarking on pseudo-real data where the true calibration map can be estimated very precisely; and (4) novel calibration and evaluation methods using new calibration map families PL and PL3.

Keywords: calibration, evaluation, classifier, ECE

1 Introduction

A classifier is considered calibrated, if in the groups of similar predictions there is an agreement with the real label distribution. Calibration is essential in safety-critical applications. Overconfident predictions can lead to costly errors,
underconfident predictions can prevent us from taking beneficial actions. In practice, a classifier’s calibration cannot be directly measured as we do not know the corresponding true probabilities for each prediction. The most common way of estimating a classifier’s calibration is through reliability diagrams and ECE (estimated calibration error, also known as the expected calibration error \(^1\)) (Murphy and Winkler, 1977; Broecker, 2011; Naeini et al, 2015). In reliability diagrams, predicted probabilities are binned together to get an estimate of the true calibrated probability in each bin by averaging the corresponding class labels. However, there is no consensus, how to place the bins in reliability diagrams and how many there should be. Usually 10, 15, or 20 bins are used (Naeini et al, 2015; Guo et al, 2017). Bins are placed with equal width, so that they take up an equal chunk in the probability space, or with equal size, so that they each contain an equal number of predictions. The choice of binning can drastically impact the shape of the reliability diagram and alter the estimated calibration error (Roelofs et al, 2020; Kumar et al, 2019; Nixon et al, 2019).

Several different solutions to this problem have been proposed: e.g. using kernel based CE estimates (Widmann et al, 2019; Zhang et al, 2020), or choosing the maximal number of bins which leads to a monotonically increasing reliability diagram (Roelofs et al, 2020). More broadly, evaluation of calibration has been the main focus of several works: Vaicenavicius et al (2019) proposed a more general definition of calibration and proposed a method to perform statistical tests of calibration, based on binning. Widmann et al (2019) proposed the kernel calibration error for calibration evaluation in multi-class classification.

The research on evaluating calibration has gone hand-in-hand with the research on post-hoc calibration, which aims to learn a calibration map transforming the classifier’s output probabilities into calibrated probabilities. Many papers contributed to both post-hoc calibration and evaluation: Naeini et al (2015) proposed BBQ and used ECE to evaluate calibration; Guo et al (2017) proposed temperature, vector and matrix scaling, and used the reliability diagrams and ECE for evaluating confidence in multi-class classification. Kumar et al (2019) proposed scaling-binning calibration, a new debiasing method for ECE and the notion of marginal calibration error. Kull et al (2019) proposed Dirichlet calibration and the notion of classwise-calibration error. Zhang et al (2020) proposed generic Mix-n-Match calibration strategies and used kernel density estimation (KDE) for estimating CE. Gupta et al (2021) proposed a calibration evaluation metric based on the Kolmogorov-Smirnov test and a calibration method based on fitting splines.

However, the existing works have not exploited the more direct link between post-hoc calibration and evaluation which we refer to as the fit-on-the-test paradigm (Section 3), stating that any post-hoc calibration method can directly be used for evaluation also. Viewing ECE as fit-on-the-test reveals its shortcomings, inspiring our proposed calibration and calibration evaluation methods PL and PL3 (Section 4).

\(^1\)Following Roelofs et al (2020), we prefer ‘estimated’ to avoid confusion with the true calibration error which involves an expectation.
Calibration evaluators can be compared based on different criteria (Section 5), and our experiments demonstrate the usefulness of the fit-on-the-test view in advancing the state-of-the-art in some of those criteria (Section 6).

2 Notation and Background

2.1 True Calibration Error

We present the methods for binary classification, but Section 2.3 shows applicability to multi-class classification as well. Consider a binary classifier \( f : \mathcal{X} \rightarrow [0, 1] \) predicting the probabilities of instances to be positive. Let \( X \in \mathcal{X} \) be a randomly drawn instance, \( Y \in \{0, 1\} \) its true class, and let us denote the model’s predictions with \( \hat{P} = f(X) \). Every classifier \( f \) has a corresponding true calibration map, which could be used to perfectly calibrate the model:

\[
c^*_f(\hat{p}) = \mathbb{E}[Y \mid \hat{P} = \hat{p}]
\]

(also known as the canonical calibration function (Vaicenavicius et al, 2019)). For evaluation of calibration, consider a test dataset with instances \( x_1, \ldots, x_n \in \mathcal{X} \) and true labels \( \bar{y}_1, \ldots, \bar{y}_n \in \{0, 1\} \), and denote the predictions by \( \hat{p}_i = f(x_i) \). The true calibration error (CE) is the model’s average violation of calibration; it could be defined on the overall test distribution as \( \mathbb{E}[| c^*_f(\hat{P}) - \hat{P}|^\alpha] \) (Kumar et al, 2019) but we define it for the test dataset:

\[
CE(\alpha) = \frac{1}{n} \sum_{i=1}^{n} | c^*_f(\hat{p}_i) - \hat{p}_i|^{\alpha}
\]

where \( \alpha = 1 \) corresponds to absolute error (MAE) and \( \alpha = 2 \) to squared error (MSE). Figure 1a shows an example of a true calibration map, where each red line shows the violation of calibration corresponding to a particular data point, and the average length of red lines equals to CE.

2.2 Reliability Diagrams and ECE

There are multiple ways to estimate calibration error. One of the most popular ways is using reliability diagrams (Murphy and Winkler, 1977). The reliability diagram is a bar plot, where each bar contains a certain region of probabilities (a bin) and the bar height corresponds to the average label (\( \bar{y}_k \)) in the \( k \)-th bin (Figure 1b). Each red line in Figure 1b shows the difference between the average label \( \bar{y}_k \) and the average prediction \( \bar{p}_k \) in the \( k \)-th bin. The vector \( \mathbf{B} = (B_1, \ldots, B_{b+1}) \) provides the bin boundaries \( 0 = B_1 < B_2 < \ldots < B_b < B_{b+1} = 1 + \epsilon \), resulting in bins \( [B_1, B_2), \ldots, [B_b, B_{b+1}) \), where \( \epsilon \) is an infinitesimal to ensure that \( 1 \in [B_b, B_{b+1}) \). Thus, \( \bar{y}_k = \frac{1}{n_k} \sum_{\hat{p} \in [B_k, B_{k+1})} y_i \) and \( \bar{p}_k = \frac{1}{n_k} \sum_{\hat{p} \in [B_k, B_{k+1})} \hat{p}_i \) where \( n_k = |\{i \mid \hat{p}_i \in [B_k, B_{k+1})\}| \) is the size of bin \( k \). The bins can be either equal size (each bin has the same number of instances), or equal width (each bin covers the equal region in the probability space).

Based on the reliability diagrams (Figure 1b), the estimated calibration error (ECE) (Naeini et al, 2015) is a weighted average between the mean
Fig. 1: (a) True calibration map (orange line) vs the predicted probabilities (dashed line). Connecting lines show instance-wise miscalibration. (b) Reliability diagram consists of bars (blue) with the height of average label. The red lines show the error between the mean labels and predicted probabilities in each bin. (c) Reliability diagram with 45-degrees tilted top lines of the bars. The diagrams are made with synthetic data (3000 data points, stratified sample of 50 data points from the bins shown for instance-wise errors, see Appendix D.3 for more details).

accuracy and the mean probability in each bin:

\[ \text{ECE}_B^{(\alpha)} = \frac{1}{n} \sum_{k=1}^{b} n_k \cdot |\bar{y}_k - \bar{p}_k|^\alpha. \]

The binning-based ECE is known to be biased (Broecker, 2011; Ferro and Fricker, 2012) with \( \mathbb{E}[\text{ECE}_B^{(\alpha)}] \neq \mathbb{E}[\text{CE}^{(\alpha)}] \), hence in our experiments we use debiasing as proposed by Kumar et al (2019).

### 2.3 Calibration Evaluation for Multi-Class

In contrast to binary classification, there are multiple different definitions of calibration for multi-class tasks:

- a binary classifier is calibrated if all predicted probabilities to be positive are calibrated: \( \Pr[Y = 1 | f(X) = \hat{p}] = \hat{p} \) for all \( \hat{p} \in [0, 1] \);
- a multi-class classifier is class-k-calibrated if all the predicted probabilities of class \( k \) are calibrated: \( \Pr[Y = k | f_k(X) = \hat{p}] = \hat{p} \) for all \( \hat{p} \in [0, 1] \) (Kull et al, 2019; Kumar et al, 2019; Nixon et al, 2019);
- a multi-class classifier is confidence calibrated if \( \Pr[Y = \text{arg max} f(X) | \max f(X) = \hat{p}] = \hat{p} \) for all \( \hat{p} \in [0, 1] \) (Kull et al, 2019; Guo et al, 2017).
However, in all of the above scenarios, we need to evaluate if the predicted and actual probabilities of an event are equal among all instances with shared predictions. By redefining \( Y = 1 \) and \( Y = 0 \) to denote whether or not the event happened and \( \hat{P} = f(X) \) to denote the estimated probability of that event, we have essentially reduced all three evaluation tasks to the first task of evaluating calibration in binary classification. The shared definition of calibration then becomes: \( \Pr[Y = 1|f(X) = \hat{p}] = \hat{p} \) or equivalently, \( \mathbb{E}[Y|f(X) = \hat{p}] = \hat{p} \). This explains also why ECE has been applied to all those 3 scenarios.

### 2.4 Post-hoc Calibration

Post-hoc calibration is the task where the goal is to use a validation set to obtain an estimate \( \hat{c} \) of the true calibration map \( c^*_f \) for a given uncalibrated classifier \( f \). Post-hoc calibration methods view the task basically as binary regression: given the predictions \( \hat{p}_1, \ldots, \hat{p}_n \in [0, 1] \) and the corresponding true binary labels \( y_1, \ldots, y_n \in \{0, 1\} \), find a ‘regression’ model \( \hat{c} : [0, 1] \to [0, 1] \) that best predicts the labels from the predictions, evaluated typically by cross-entropy or mean squared error which in this context are respectively known as the log-loss and the Brier score - two members of the family of strictly proper losses (Brier, 1950). **Why are proper losses a good way of evaluating progress towards estimating the true calibration map?** A common justification is that these losses have the virtue that they are minimised by the perfectly calibrated model \( c^*_f \) (Kumar et al, 2019), that is: \( \arg\min_{\hat{c}(\hat{p})} \mathbb{E}[l(\hat{c}(\hat{p}), Y)|\hat{P} = \hat{p}] = c^*_f(\hat{p}) \) for any \( \hat{p} \in [0, 1] \) and any strictly proper loss \( l \). However, this justification refers to the optimum only. Our following Theorem 1 makes even a stronger claim that a reduction of the expected loss \( l \) leads to the same-sized improvement in how well \( \hat{c}(\hat{p}) \) approximates \( c^*_f(\hat{p}) \), measured by any Bregman divergence \( d : [0, 1] \to [0, 1] \) (here \( d \) quantifies similarity between two binary categorical probability distributions, and it is a strictly proper loss when the label is its second argument, see details and proofs of the theorems in Appendix B):

**Theorem 1** Let \( d : [0, 1] \times [0, 1] \to \mathbb{R} \) be any Bregman divergence and \( \hat{c}_1, \hat{c}_2 : [0, 1] \to [0, 1] \) be two estimated calibration maps. Then

\[
\mathbb{E}[d(\hat{c}_1(\hat{p}), Y)|\hat{P} = \hat{p}] - \mathbb{E}[d(\hat{c}_2(\hat{p}), Y)|\hat{P} = \hat{p}] = d(\hat{c}_1(\hat{p}), c^*_f(\hat{p})) - d(\hat{c}_2(\hat{p}), c^*_f(\hat{p})).
\]

The above theorem involves expectations conditioned on \( \hat{p} \) which are typically impossible to estimate for any particular \( \hat{p} \) in isolation, because there is just one or very few instances with exactly the same predicted probability \( \hat{p} \). Therefore, most post-hoc calibration methods minimize the empirical loss \( \sum_{i=1}^n d(\hat{c}(\hat{p}_i), y_i) \) for \( \hat{c} \) in some sub-family \( \mathcal{C} \) within all possible calibration maps, using inductive biases such as assuming \( c^*_f \) is monotonic (isotonic calibration (Zadrozny and Elkan, 2002)), or belongs to some parametric family, e.g. logistic functions (Platt scaling (Platt, 2000)).
3 The Fit-on-the-Test Paradigm

3.1 Fit-on-the-Test Calibration Evaluation

Looking at the challenges of choosing a good binning for ECE and the existing attempts of improving over ECE, we asked ourselves: what are the ways of extending the toolkit of evaluation methods for calibration. We realized that there is a simple way to obtain a new evaluation method starting from any strictly proper loss $l$ and any family $C$ of calibration map functions. For different choices of $l$ and $C$ we obtain a rich family of methods which we refer to as fit-on-the-test evaluation methods. These methods fit the family $C$ on the test set by minimizing $l$, obtaining an estimate $\hat{c}$ of the true calibration map $c_f^*$:

$$\hat{c}_{\text{fit-on-the-test}} = \arg\min_{c \in C} \frac{1}{n} \sum_{i=1}^{n} l(c(\hat{p}_i), y_i).$$

We refer to this function as the fit-on-the-test reliability diagram. We call it a reliability diagram because similarly to the classical binning-based reliability diagrams, it maps predicted probabilities to empirically calibrated probabilities. Essentially, the fit-on-the-test reliability diagram is obtained by post-hoc calibration on the test set. Based on this diagram, the calibration error is directly estimated as follows:

$$\text{ECE}^{(\alpha)}_{\text{fit-on-the-test}} = \frac{1}{n} \sum_{i=1}^{n} |\hat{c}_{\text{fit-on-the-test}}(\hat{p}_i) - \hat{p}_i|^\alpha.$$

We refer to this estimate as the fit-on-the-test calibration measure.

Since almost all post-hoc calibration methods are based on fitting some family $C$, adopting the fit-on-the-test principle opens up opportunities in using any of those families for evaluating calibration also. For example, our experiments in Section 6 show that the fit-on-the-test reliability diagrams corresponding to the families of isotonic calibration, Platt scaling or beta calibration are typically closer to the true calibration map than the classical binning-based reliability diagrams.

Why has the fit-on-the-test view on evaluation not been exploited before? We guess this is due to the following potential concerns:

1. Due to inevitable overfitting (or the generalisation gap) in any fitting process, we are bound to get our estimated $\hat{c}$ closer to the observed labels than $c_f^*$ is, hence harming our capability of estimating the true calibration error $|c_f^*(\hat{p}) - \hat{p}|$.
2. By choosing a particular family $C$ of functions to be used during the fitting process, we would misjudge the calibration error in the cases where $c_f^*$ is not in this family.

It seems impossible to fully solve both problems at the same time: a more restrictive set of functions helps against overfitting and alleviates the first
problem, but increases the second problem; a bigger set of functions helps against the second problem, but increases overfitting. However, our experiments demonstrate that good tradeoffs are possible, using flexible families but still with relatively few parameters.

The classical binning-based ECE might seem to sidestep this problem and instead of estimating $c_f^*$ at all given points, it performs the comparison of bin averages $\bar{p}$ and $\bar{y}$. Perhaps surprisingly though, it is possible to show that the binning-based ECE can also be seen as a fit-on-the-test calibration measure for a particular family of functions $\mathcal{C}$ with the Brier score (MSE) as the loss function, and thus the above concerns are valid for the standard ECE as well.

Before demonstrating this, we first introduce a bigger family $\mathcal{C}(b)_{B,H,A}$ of (typically) non-continuous, piecewise linear functions, parametrised by the boundaries of the $b$ pieces (or bins) denoted as $B \in [0,1]^{b+1}$ for some number of bins $b \in \mathbb{N}$, values of the function at the boundaries $B_1, \ldots, B_b$ denoted as $H \in [0,1]^b$, and by the slopes of linear functions within the bins, denoted as $A \in \mathbb{R}^b$:

$$c(B,H,A)(\hat{p}) = \sum_{k=1}^{b} I[B_k \leq \hat{p} < B_{k+1}] \cdot (H_k + A_k(\hat{p} - B_k))$$

where $I[\cdot]$ is the indicator function. As when defining the reliability diagrams, the bin boundaries are here also restricted to satisfy $0 = B_1 < B_2 < \ldots < B_b < B_{b+1} = 1 + \epsilon$. Note that the resulting functions can be non-continuous because the right side of the bin $[B_k, B_{k+1})$ ends near the value $H_k + A_k(B_{k+1} - B_k)$ and nothing is preventing this value from being different than $H_{k+1}$ which is the left side of the bin $[B_{k+1}, B_{k+2})$.

It turns out that the classical binning-based ECE is a fit-on-the-test calibration measure with respect to a particular subfamily of $\mathcal{C}(b)_{B,H,A}$ that we will describe next. As ECE is calculated from the reliability diagrams that are piecewise constant, one might guess that this subfamily would contain all the piecewise constant (slope 0) functions with a particular fixed binning $B$. However, ECE with the binning $B$ is actually a fit-on-the-test calibration measure with respect to the subfamily $\mathcal{C}(b)_{B,1}$ which contains functions with slope 1 (i.e. a 45-degrees ascending slope) in each of the bins. That is, $\mathcal{C}(B,1)$ contains all functions with the fixed binning $B$, fixed slopes $A = 1 = (1,1,\ldots,1)$ with $|1| = b$, and any heights $H \in \mathbb{R}^b$ for the left-side boundaries of these bins. Figure 1 illustrates this, showing that each of the bin-specific red lines marking the calibration gaps $|\bar{p}_k - \bar{y}_k|$ in Figure 1b can be split into multiple instance-specific red lines $|\hat{c}(\hat{p}_i) - \hat{p}_i|$ with the same length in Figure 1c. The lengths are equal because the diagonal and the top of the bin have both slope 1. Thus, the average length of red gap lines in Figure 1c is exactly equal to the bin-size-weighted average of red gap lines in Figure 1b, that is the classical binning-based ECE. The following theorem proves that this equality is indeed achieved by fitting $\mathcal{C}(B,1)$:
Theorem 2 Consider a predictive model with predictions \( \hat{p}_1, \ldots, \hat{p}_n \in [0, 1] \) on a test set with actual labels \( y_1, \ldots, y_n \) and a binning \( B \) with \( b \geq 1 \) bins and boundaries \( 0 = B_1 < \cdots < B_{b+1} = 1 + \epsilon \). Then for any \( \alpha > 0 \), the measure \( \text{ECE}^{(\alpha)}_B \) is equal to:

\[
\text{ECE}^{(\alpha)}_B = \frac{1}{n} \sum_{i=1}^{n} |\hat{c}(\hat{p}_i) - \hat{p}_i|^\alpha
\]

where \( \hat{c} = \arg\min_{c \in C_{(B,H,1)}} \frac{1}{n} \sum_{i=1}^{n} (c(\hat{p}_i) - y_i)^2 \).

Furthermore, \( \hat{c}(\bar{\hat{p}}_k) = \bar{y}_k \) for \( k = 1, \ldots, b \), where \( \bar{\hat{p}}_k \) and \( \bar{y}_k \) are the average \( \hat{p}_i \) and \( y_i \) in the bin \([B_k, B_{k+1})\).

The resulting new tilted-roof reliability diagrams as in Figure 1c are the same as the standard ones as in Figure 1b except for the tilted tops. However, as a result, it is easier to visually assess the amount of miscalibration. For example, if the distribution of the predictions were uniform within \([0, 1]\), then the area between the tilted-roof reliability diagram and the diagonal would be equal to ECE. In contrast, for the classical reliability diagrams the value of ECE can not be assessed from the bars, but only from the gaps (red bars in Figure 1b) and even then only if the gaps are drawn with the x-axis location at \( \bar{\hat{p}}_k \) instead of bin centres. For example, the leftmost bar in Figure 1b corresponds to the bin \([0, 0.1)\) and has height \( \bar{y}_k = 0.08 \) with a gap of 0.06 to the average prediction of \( \bar{\hat{p}}_k = 0.02 \). However, if the red bar were not shown or were wrongly drawn at the centre of the bar, then the amount of calibration error could not be assessed from the figure. Furthermore, a perfectly calibrated model with \( \bar{y}_k = \bar{\hat{p}}_k = 0.08 \) would have the leftmost blue bar identical to the current one, and only the zero-height red gap bar could reveal that it is actually calibrated. In contrast, there is no need to show the gaps in the tilted-roof reliability diagrams, because the height difference of the bar from the diagonal is equal to the estimated calibration error within this bin.

3.2 Cross-Validated Number of Bins for ECE

Viewing the binning-based \( \text{ECE}^{(\alpha)}_B \) as fitting the family \( C^{(b)}_{(B,H,1)} \) on the test data, we can see the choice of the number of bins \( b \) as a hyper-parameter optimisation task. We can now come up with novel methods for choosing the number of bins for ECE. For example, we can split the test set randomly into two folds: on one fold we perform fitting with different numbers of bins, and on the other fold evaluate which number of bins provides the best fit. After that, the final reliability diagram could be drawn with this selected number of bins, and ECE calculated based on this diagram. Instead of such fixed split into two folds, any other hyper-parameter optimisation technique can be used. We propose to use cross-validation (CV), a typical hyper-parameter tuning method, to select the number of bins which provides the best fit (Figure 2a). Note that we are fitting \( \hat{c}(\hat{p}_i) \) to \( y_i \) for \( i = 1, \ldots, n \) and thus CV is improving the fit between the tilted tops of the reliability diagram and the binary labels.
As a result, the fit between the estimated calibration function \( \hat{c} \) (the tilted tops of the reliability diagram) and the true calibration curve \( c^*_f \) also improves in expectation, as implied by Theorem 1. A better fit of \( \hat{c} \) and \( c^*_f \) implies a ‘more reliable’ reliability diagram, in the sense that on average, each point at the top of the bars is on average closer to the true calibration function. While cross-validation is a standard tool for hyperparameter tuning, it has been missed for ECE because it has not been seen as fitting before.

In the implementation of CV, inspired by Tikka and Hollmén (2008), we prefer a lower number of bins whenever the relative difference in loss is less than 0.1 percent, further improving performance (for details see Appendix C.2).

4 Calibration Map Families PL and PL3

4.1 PL - Piecewise Linear Calibration Maps

The family \( \mathcal{C}^{(b)}_{(B,H,1)} \) of functions used by the binning-based ECE has several weaknesses: (1) it contains non-continuous functions while ‘jumps’ are unlikely to be present in the true calibration function; (2) it only contains segments with slope 1, making it hard to fit the true calibration function in regions with a different slope.

Therefore, we are instead looking for a family satisfying the following criteria: (1) contains only continuous functions; (2) has flexibility to fit any curve; (3) contains the identity function; (4) has few parameters not to overfit heavily. We propose to use the subfamily \( \mathcal{C}^{(b)}_{B,H,\text{cont}} \) of continuous functions from the piecewise linear function family \( \mathcal{C}^{(b)}_{B,H,A} \). The family \( \mathcal{C}^{(b)}_{B,H,\text{cont}} \) is only parametrised by the bin boundaries \( B \) and by the values \( H \) of the function at the boundaries, whereas the slopes can be calculated from \( B \) and \( H \) with...
A_k = \frac{H_{k+1} - H_k}{B_{k+1} - B_k} \text{ to ensure that the line at the right end of bin } k \text{ coincides with the line at the left end of bin } k + 1. \text{ Note that the bin boundaries } B \text{ are now also parameters to be fitted, together with the values } H. \text{ As } B_1 = 0 \text{ and } B_{b+1} = 1 + \epsilon \text{ are fixed, we are fitting } 2b \text{ parameters: } b - 1 \text{ bin boundaries and } b + 1 \text{ values in } H. \text{ The number of bins } b \text{ is optimised through cross-validation, similarly to Section 3.2.}

We call the corresponding fit-(C_{B,H,cont,l})-on-the-test method as PL: the piecewise linear method for evaluating calibration. In particular, we can now draw new kind of piecewise linear reliability diagrams (Figure 2b) which provide a better fit to the true calibration function than the binning-based methods, as demonstrated in our experiments (Section 6). For a visual comparison, check Figure 2a and Figure 2b, as these figures have been made with the same data. More comparative examples can be found in Appendix E.1. Therefore, the piecewise linear reliability diagram can be used similarly to the classical ECE reliability diagram to check visually how well the model is calibrated. We can then also estimate the calibration error as a single number ECE_{PL} which we call the piecewise linear ECE or in short ECE_{PL}. ECE_{PL} measures the instance-wise average distance from the piecewise linear function to the main diagonal:

\begin{equation}
ECE_{PL} = \frac{1}{n} \sum_{i=1}^{n} |\hat{c}(\hat{p}_i) - \hat{p}_i|^\alpha \text{ where } \hat{c} = \arg\min_{c} C_{B,H,cont}(B,H,cont,\hat{p}_i, y_i, 2).
\end{equation}

**Implementation Details**

Although the continuous piecewise linear functions are mathematically very well known, we found only one existing public implementation (Jekel and Venter, 2019), based on least squares fitting with differential evolution. We included this in our experiments with the name PL_{DE} (results in Appendix F). However, we also created ourselves a neural network based implementation depicted in Figure 3, which allowed us to add cross-entropy fitting. Full details about the architecture are given in Appendix C, but here is a short overview.

We have a single input (\hat{p}) and a single output (\hat{c}) connected through two layers: the binning layer and the interpolation layer. The binning layer has \( b + 1 \) gating units corresponding to the bin boundaries, each outputting whether \( \hat{p} \) is to the left or to the right of the boundary. The binning layer is parametrised by \( b \) real values which are passed through the softmax (\( \sigma \)) to obtain the widths of the bins and through cumulative sum (\( B_i = \sum_{k=1}^{i} \sigma_k(B) \)) to obtain bin boundaries. These parameters are initialised such that all bins contain the same number of training instances. The interpolation layer has \( b + 1 \) parameters which are each passed through the logistic function (\( \phi \)) to obtain the calibration map values \( H_1, \ldots, H_{b+1} \) at the bin boundaries. These are initialised such that the represented calibration map is the identity function. The \( b \) units correspond to the bins and the bin to which \( \hat{p} \) belongs produces the linearly interpolated output. Based on these values, the piecewise linear function value is calculated...
We use 10-fold-cross-validation to select the number of segments in the piecewise linear function to best approximate the true calibration map, similar to Section 3.2. The same way as in hyperparameter optimization for Dirichlet calibration Kull et al (2019), the predictions on test data are obtained as an average output from all the 10 models with the chosen number of segments but trained from different folds, i.e. we are not refitting a single model on all 10 folds.

4.2 PL3 - Piecewise Linear in Logit-Logit Space

When evaluating calibration of neural networks, it makes sense to look for calibration map families that have been successfully used for post-hoc calibration. Thus, we consider temperature scaling, fitting a family of functions $\hat{c}(\hat{p}) = \sigma(z/t)$ with a single temperature parameter $t$, where the softmax $\sigma$ is applied on logits $z$ that the uncalibrated model would have directly converted into probabilities with $\hat{p} = \sigma(z)$ (Guo et al, 2017). In the binary classification case with a single output, $\sigma(z) = 1/(1 + e^{-z})$ is the logistic function, the inverse function of the logit $\sigma^{-1}(p) = \ln(p/(1 - p))$. Importantly, if plotted
in the logit-logit scale, binary temperature scaling fits a straight line, since
\[ \sigma^{-1}(\hat{c}(\hat{p})) = \sigma^{-1}(\sigma(z/t)) = z/t = 1/t \cdot \sigma^{-1}(\sigma(z)) = \sigma^{-1}(\hat{p}). \]

Interestingly, another post-hoc calibration method known as beta calibration (Kull et al, 2017) fits calibration maps which in the logit-logit space are approximately piecewise linear with two segments, as shown in Figure 4 (top right subfigure, blue line). The proof for this fact is given in Appendix E.2. This motivates our calibration map family PL3 of Piecewise Linear functions in the Logit-Logit space (PLL\(_L=PL3\)), which corresponds to temperature scaling when using 1 piece, approximates beta calibration when using 2 pieces, and can take more complicated shapes when using more linear pieces in the logit-logit space. On Figure 2c is an example of a piecewise linear in logit-logit space reliability diagram. Further details are provided in Appendix E.2.

**Implementation Details**

We use the same neural architecture as for PL, except that the expected input is in the logit space, the bin boundaries are converted into the logit space, the logistic is removed from the parameters feeding the interpolation layer, and instead the logistic is applied on the final output. Further details are given in Appendix C.

5 Assessment of Calibrators and Evaluators

5.1 Assessment of Post-hoc Calibrators

Before proceeding to the experiments, let us discuss the methods for assessing the quality of calibrators and evaluators of calibration. Post-hoc calibrators should be evaluated based on the effectiveness of calibration, but this effectiveness could be interpreted in two ways. Firstly, we could evaluate how well-calibrated the outputs of the calibrator are by calculating the calibration error after calibration (CEAC):

\[ CEAC = CE(\hat{c} \circ f) = E[d(\hat{C}, c^*_{\hat{c} \circ f}(\hat{C}))] \]

Secondly, we could evaluate how well the calibrator approximates the true calibration map by calculating the calibration map estimation error (CMEE):

\[ CMEE = E[d(\hat{c}(\hat{P}), c^*_f(\hat{P}))] \]

where \( d \) is any Bregman divergence and \( \hat{C} = \hat{c}(\hat{P}) = (\hat{c} \circ f)(X) = \hat{c}(f(X)) \). We prove that low calibration map estimation error is a stronger requirement than low calibration error after calibration, because \( CMEE \) is an upper bound for \( CEAC \):

**Theorem 3**

\[ CMEE = CEAC + E[d(c^*_{\hat{c} \circ f}(\hat{C}), c^*_f(\hat{P}))]. \]
Fig. 4: Motivation for PL3. Comparison of results in the probability space (left column) and in the logit-logit space (right column). Methods are split into two groups for clarity. In essence, sub-figures (a) and (b) are the same, only display different functions. Model ResNet110 (He et al, 2015) on "cats vs rest" task of CIFAR-5m.

Intuitively, the difference between CMEE and CEAC is due to ties introduced by \( \hat{c} \) where \( \hat{c}(\hat{p}) = \hat{c}(\hat{p}') \) while \( c_f^*(\hat{p}) \neq c_f^*(\hat{p}') \) for some \( \hat{p} \neq \hat{p}' \). As low CMEE is a stronger requirement, we prefer this measure in the experiments. We use the notation \( d(\hat{c}, c^*) \) as a more memorable synonym for CMEE.
5.2 Assessment of Calibration Evaluators

Calibration evaluators that follow the fit-on-the-test paradigm, estimate $\hat{c}$ on the test data. The resulting $\hat{c}$ can be viewed as a reliability diagram, or used to estimate the calibration error with $ECE_{\text{fit-(C, l)-on-the-test}}^{(\alpha)}$.

We see 3 main application scenarios:

1. the reliability diagram is needed if the downstream decision-making process performed by a human or AI requires information about the extent to which different probabilistic predictions can be trusted;
2. the estimated calibration error is needed if the general level of trust needs to be known, not specifically for each output;
3. and the ranking of the estimated calibration errors is needed if performing selection of the best calibrated model.

In the experiments, we evaluate each calibration evaluation method $\mathcal{M}$ against these three objectives, measuring: (1) the quality of reliability diagrams with $d(\hat{c}_M, c^*)$; (2) the quality of calibration error estimates with $|ECE_M - CE|$; and (3) the quality of ranking performance using Spearman’s correlation of the ranking produced by the calibration evaluator against the ranking of true calibration errors, which we refer to as $\text{rankcorr}(ECE_M, CE)$. All these methods assume good estimates of the true calibration map, which can be obtained either on synthetic data or if there is access to magnitudes of more data than the calibration evaluator used.

Note that in the experiments we mostly use the absolute difference $d(\hat{c}, c^*) = |\hat{c} - c^*|$ as the distance measure between the estimated and true calibration maps, following the tradition of how ECE is calculated from the reliability diagrams. As the absolute difference is not a Bregman divergence, the Appendix also considers the squared difference $d(\hat{c}, c^*) = |\hat{c} - c^*|^2$ which is a Bregman divergence. Importantly, a method $\mathcal{M}$ that produces the best calibration map estimate with the lowest $|\hat{c}_M - c^*|$ might not be the same as method $\mathcal{M}'$ that produces the best calibration error estimate $|ECE_{\mathcal{M}'} - CE|$. For example, this occurs when comparing the methods in Figures 2a and 2b. In Figure 2b, the piecewise linear method (PL) achieves $|ECE_{PL} - CE| = 0.0045$ and $|\hat{c}_{PL} - c^*| = 0.0204$, while in Figure 2a, equal-width binning with cross-validated number of bins ($EW_{CW}$) achieves $|ECE_{EW_{CV}} - CE| = 0.0024$ and $|\hat{c}_{EW_{CV}} - c^*| = 0.0398$. Thus, even though PL has in this example better $|\hat{c} - c^*|$, it still loses to $EW_{CV}$ with respect to $|ECE - CE|$. Intuitively, $EW_{CV}$ has bigger errors in the reliability diagram, but during the calculation of ECE these errors happen to cancel out more than in the case of PL.

6 Experiments and Results

The goal of our experimental studies is to (1) evaluate our proposed PL and PL3 calibration map families as calibration methods; and (2) find the best calibration map family for calibration evaluation (thanks to the fit-on-the-test paradigm).
Table 1: Comparison of post-hoc calibrators with respect to $|\hat{c}_M - c^*| \times 10^3$ in estimating the true calibration map of DenseNet40, ResNet110 and WideNet32 classifiers on CIFAR-5m. Calibrators are trained on 5000 instances, results are averaged across the 3 classifiers.

| Method                  | Platt | beta | isotonic | ScaleBin | TempS | 1-Temp | VecS | dirL2 | dirODIR | MSODIR | Spline | IOP | ES$_{sweep}$ | PL3 | PL |
|-------------------------|-------|------|----------|----------|-------|--------|------|-------|--------|--------|-------|-----|-------------|-----|----|
| cars vs rest            | 3.8t  | 4.3t | 4.0t     | 4.4t     | 7.3t  | 5.0t   | 4.8t | 5.6t  | 3.8t   | 4.3t   | 6.7t  | 8.2t | 7.1t        | 2.9t | 5.0t |
| dogs vs rest            | 4.5t  | 14.1t| 8.6t     | 6.7t     | 11.7t | 6.9t   | 8.6t | 12.7t | 11.6t  | 11.5t  | 8.7t  | 11.0t| 10.5t       | 5.3t | 12.3t|
| confidence              | 13.1t | 17.4t| 11.6t    | 8.7t     | 22.7t | 30.9t  | 34.2t| 40.9t | 38.1t  | 37.5t  | 15.4t| 24.8t| 29.9t       | 8.5t | 15.4t|

A key problem for research in calibration evaluation methods and post-hoc calibration methods is that proper evaluation requires access to the true calibration map. This, however, is unknown. One workaround would be to use synthetically created data, where the true calibration map is known. However, with synthetic data the shape of the true calibration map might not be realistic.

Our solution to this is to use the pseudo-real dataset CIFAR-5m (Nakkiran et al., 2021) with 5 million synthetic images, created such that the models trained on CIFAR-10 (Krizhevsky et al., 2009) have very similar performance on CIFAR-5m, and vice versa. Thus, it is likely that the true calibration maps are also very realistic. Thanks to the vast size of the CIFAR-5m dataset we can estimate the true calibration map very precisely. In our experiments, we used isotonic calibration on 1 million hold-out datapoints to estimate the true calibration map (other options than isotonic were considered in Appendix F, minor differences in the results). The main part of the experiments concentrates on CIFAR-5m, while Appendix F shows more results on synthetic and real datasets, where the results are comparable to CIFAR-5m with minor differences, supporting the overall conclusions. On CIFAR-5m, we concentrated on three 1-vs-rest calibration tasks (car, cat, dog) and confidence calibration. Only three 1-vs-rest tasks were used due to computational limitations.

ResNet110 (He et al., 2015), WideNet32 (Zagoruyko and Komodakis, 2016) and DenseNet40 (Huang et al., 2016) models were trained on 45k datapoints from CIFAR-5m, additional 5k datapoints were used to calibrate the outputs of models with multi-class calibration methods: temperature scaling (TempS), vector scaling (VecS), and matrix scaling with off-diagonal and intercept regularisation (MSODIR); Dirichlet calibration with L2 and ODIR regularisation (dirL2/dirODIR), Spline with natural method (Spline); Order-invariant version of intra-order preserving functions (IOP); binary calibration methods: Platt, isotonic, beta calibration (beta), temperature scaling for binary calibration (1-Temp), scaling-binning (ScaleBin), ECE-based binning (ES$_{sweep}$) methods with equal-size binning (ES), piecewise linear methods (PL and PL3). For PL we used our neural network model trained with cross-entropy loss (the results with optimising for Brier score and with the alternative optimisation method based on differential evolution are included in Appendix F).

The source code for conducting the experiments is available at https://github.com/markus93/fit-on-the-test.
We show the results in absolute differences (i.e. $\sum_{i=1}^{n} |\hat{c}_M - c^*|$) on CIFAR-5m. In contrast to Table 1, the evaluators are compared on predictions that have been previously post-hoc calibrated.

| Task | Initial model | Data size | ES_{sweep} | ES_{CV} | PL3 | PL | Platt | beta | isotonic | Spline | IOP |
|------|---------------|-----------|------------|---------|-----|----|-------|------|---------|--------|-----|
| cars vs rest | ResNet110 | 1000 | 13.34 | 11.44 | 11.19 | 10.23 | 8.02 | 10.88 | 9.63 | 12.99 | 12.08 | 8.17 |
| cats vs rest | DenseNet40 | 1000 | 8.46 | 7.64 | 8.19 | 6.64 | 6.22 | 7.44 | 6.83 | 8.65 | 9.24 | 7.43 |
| dogs vs rest | WideNet32 | 10000 | 6.61 | 6.77 | 5.88 | 4.92 | 4.59 | 6.85 | 6.88 | 5.97 | 7.34 | 7.81 |
| confidence | ES | All | 9.47 | 8.62 | 8.52 | 7.27 | 6.27 | 8.39 | 7.63 | 9.24 | 9.55 | 7.81 |

Results

We show the results in absolute differences (i.e. $\alpha = 1$) as in most earlier works (Appendix F has the quadratic also, i.e. $\alpha = 2$). Table 1 assesses PL and PL3 as post-hoc calibration methods. The calibration map family corresponding to ECE fit with the sweeping method Roelofs et al (2020) is also included as $ES_{sweep}$. The calibration methods are evaluated by how well they approximate the true calibration map: $|\hat{c}_M - c^*| = \sum_{i=1}^{n} |\hat{c}_M(\hat{p}_i) - c^*(\hat{p}_i)|$ is measured on unseen 1 million data points against the ground truth, where $\hat{p}_i$ are the outputs of the classifier, $\hat{c}_M(\hat{p}_i)$ are the post-hoc calibrated predictions, and $c^*(\hat{p}_i)$ is the ‘true’ calibration map. PL3 is the best method in all cases, showing the usefulness of the logit-logit space when calibrating neural models which are far from being calibrated. Appendix F includes more variations of these methods, the KDE method and results for each architecture separately (minor differences).

Next we compare the calibration evaluators against each of the 3 objectives listed in Section 5.2. We perform the comparison in tasks where the models are already quite close to being calibrated, because this is typical when evaluators are used for finding out which post-hoc calibrator is performing best. We compare evaluators in the task of evaluating 6 post-hoc calibrators: we measure how precisely the evaluators $M$ estimate the reliability diagrams (Table 2 showing $|\hat{c}_M - c^*|$), the total true calibration errors (Table 3 showing $|ECE_M - CE|$), and how well the estimated ranking of 6 calibrators agrees with the true ranking based on true calibration errors (Table 3 showing rankcorrel($ECE_M, CE$)). The 6 calibrators were chosen as the best methods from Table 1: beta, vector scaling, Platt, PL3, scaling-binning, isotonic. The evaluators are compared on different test set sizes 1k, 3k, 10k with 5 different random seeds for each size.

The first objective is to assess the reliability diagrams using $|\hat{c}_M - c^*| = \sum_{i=1}^{n} |\hat{c}_M(\hat{p}_i) - c^*(\hat{p}_i)|$ measured on 1 million unseen data points, where $\hat{p}_i$ are now the already post-hoc calibrated outputs of the classifier (calibrated with the 6 best methods from Table 1 trained on 5k data points), $\hat{c}_M(\hat{p}_i)$ are the
Table 3: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_M - CE|$ ($\times 10^3$) and the ranking of 6 calibrators with rankcorrel($ECE$) on CIFAR-5m.

| Metric | Data       | $ES_{15}$ | $ES_{\text{sweep}}$ | $ES_{\text{CV}}$ | $PL_3$ | $PL$   | Platt | isotonic | Spline | IOP |
|--------|------------|-----------|---------------------|-----------------|--------|--------|-------|----------|--------|-----|
| $|ECE_M - CE|$ | one-vs-rest | 2.34      | 3.24                | 3.69             | 3.59   | 2.87   | 3.63  | 3.94     | 4.06   | 3.89|
|        | confidence | 4.54      | 5.14                | 6.37             | 4.73   | 5.24   | 5.83  | 4.39     | 7.20   | 7.39|
| rankcorrel($ECE$) | one-vs-rest | 0.45      | 0.19                | 0.44             | 0.36   | 0.54   | 0.19  | 0.12     | 0.55   | -0.04|
|        | confidence | 0.62      | 0.43                | 0.56             | 0.40   | 0.51   | 0.01  | 0.51     | 0.65   | -0.05|

The results of fit-on-the-test calibration applied on top of the post-hoc calibrated predictions (trained on another separate data set of size either 1k, 3k, or 10k), and $c^*(\hat{p}_i)$ is the ‘true’ calibration map of the post-hoc calibrated predictions.

The results in Table 2 show that PL is the best on average, as well as after disaggregating according to the classifier’s architecture, test set size, or the task. PL3 is mostly second and the evaluator using the beta calibration map family is mostly third. The order invariant version of IOP shows also promising results. The performance of beta calibration varies with the size of the test dataset. This is expected, because this method has only 3 parameters which is good for small test sets but worse for bigger test sets. Similarly, the data set size affects IOP too, again because of the small number of parameters. The methods based on equal-size binning are performing worse, with $ES_{\text{CV}}$ ranking the highest on average, closely followed by $ES_{\text{sweep}}$, and the classical $ES_{15}$ with 15 bins lagging behind. Further, the Spline method is among one of the worst performing methods. From Table 1 and Table 2 we can conclude that when predictions are far from being calibrated then PL3 is best for approximating the true calibration map, and PL is best when predictions are nearly calibrated. Appendix F discusses the results showing different aggregations, and reports the optimal numbers of bins for ES and PL methods.

The second objective is to estimate the numeric value of the total true calibration error, and here the rows $|ECE_M - CE|$ of Table 3 show the benefits of $ES_{15}$, beta calibration and PL3 (with some differences across tasks). This demonstrates that while the tilted-top reliability diagrams of $ES_{15}$ are not precise, their debiased average distance from the diagonal closely agrees with the average distance of the true reliabilities (true calibration map) from the diagonal. While PL and PL3 perform reasonably well, there is a big potential for further improvements, because debiasing remains as future work for these methods. The ranking of 6 calibrators is best done by the isotonic fit-on-the-test evaluator, achieving over 55% correlation to the true ranking for one-vs-rest tasks and over 65% for the confidence task.

7 Conclusion and Future Work

We suggest to view evaluation of calibration according to the fit-on-the-test paradigm, promoting the use of post-hoc calibration methods for calibration evaluation. This view enables reliability diagrams that are closer to the true
calibration maps, more exact estimates of the total calibration error, and ranking of calibrators in the order which better corresponds to their true quality. Following fit-on-the-test, we have proposed cross-validation to tune the number of bins in ECE, and demonstrated the benefits of piecewise linearity in the original as well as in the logit-logit space, inspired by temperature scaling and beta calibration.

Future work involves development of debiasing methods for $ECE_{PL}$ and $ECE_{PL3}$, and analysing further the benefits of different calibration map families in different scenarios, including dataset shift.

Acknowledgments. This work was supported by the Estonian Research Council grant PRG1604 and by the European Social Fund via IT Academy programme.

References

Brier GW (1950) Verification of forecasts expressed in terms of probability. Monthly Weather Review 78(1):1–3

Broecker J (2011) Estimating reliability and resolution of probability forecasts through decomposition of the empirical score. Climate Dynamics 39:655–667

Ferro C, Fricker TE (2012) A bias-corrected decomposition of the brier score. Quarterly Journal of the Royal Meteorological Society 138:1954–1960

Guo C, Pleiss G, Sun Y, et al (2017) On Calibration of Modern Neural Networks. In: Thirty-fourth International Conference on Machine Learning, Sydney, Australia, URL http://arxiv.org/abs/1706.04599, 1706.04599

Gupta K, Rahimi A, Ajanthan T, et al (2021) Calibration of neural networks using splines. In: International Conference on Learning Representations, URL https://openreview.net/forum?id=eQe8DEWNN2W

He K, Zhang X, Ren S, et al (2015) Deep residual learning for image recognition. CoRR abs/1512.03385. URL http://arxiv.org/abs/1512.03385, https://arxiv.org/abs/1512.03385

Ho J, Jain A, Abbeel P (2020) Denoising diffusion probabilistic models. arXiv preprint arxiv:200611239

Huang G, Liu Z, Weinberger KQ (2016) Densely connected convolutional networks. CoRR abs/1608.06993. URL http://arxiv.org/abs/1608.06993, https://arxiv.org/abs/1608.06993

Jekel CF, Venter G (2019) pwlf: A Python Library for Fitting 1D Continuous Piecewise Linear Functions. URL https://github.com/cjekel/piecewise_linear_fit_py
Kingma DP, Ba J (2014) Adam: A method for stochastic optimization. arXiv preprint arXiv:14126980

Krizhevsky A, Hinton G, et al (2009) Learning multiple layers of features from tiny images

Kull M, Silva Filho T, Flach P (2017) Beta calibration: a well-founded and easily implemented improvement on logistic calibration for binary classifiers. In: Singh A, Zhu J (eds) Proceedings of the 20th International Conference on Artificial Intelligence and Statistics, Proceedings of Machine Learning Research, vol 54. PMLR, Fort Lauderdale, FL, USA, pp 623–631

Kull M, Perelló-Nieto M, Kängsepp M, et al (2019) Beyond temperature scaling: Obtaining well-calibrated multiclass probabilities with dirichlet calibration. In: Advances in Neural Information Processing Systems (NeurIPS)

Kumar A, Liang P, Ma T (2019) Verified uncertainty calibration. In: Advances in Neural Information Processing Systems (NeurIPS’19)

Murphy AH, Winkler RL (1977) Reliability of subjective probability forecasts of precipitation and temperature. Journal of the Royal Statistical Society Series C (Applied Statistics) 26(1):41–47

Naeini MP, Cooper G, Hauskrecht M (2015) Obtaining well calibrated probabilities using bayesian binning. In: AAAI Conference on Artificial Intelligence

Nakkiran P, Neyshabur B, Sedghi H (2021) The deep bootstrap framework: Good online learners are good offline generalizers. 2010.08127

Nieto MP, Song H, Filho TS, et al (2019) PyCalib: Python library for classifier calibration. URL https://github.com/classifier-calibration/PyCalib

Nixon J, Dusenberry M, Zhang L, et al (2019) Measuring calibration in deep learning. ArXiv abs/1904.01685

Platt J (2000) Probabilities for SV machines. In: Smola A, Bartlett P, Schölkopf B, et al (eds) Advances in Large Margin Classifiers. MIT Press, p 61–74

Rahimi A, Shaban A, Cheng CA, et al (2020) Intra order-preserving functions for calibration of multi-class neural networks. In: Advances in Neural Information Processing Systems (NeurIPS)

Roelofs R, Cain N, Shlens J, et al (2020) Mitigating bias in calibration error estimation. ArXiv abs/2012.08668

Tikka J, Hollmén J (2008) Sequential input selection algorithm for long-term prediction of time series. Neurocomputing 71(13):2604–2615. https:
Vaicenavicius J, Widmann D, Andersson C, et al (2019) Evaluating model calibration in classification. In: Chaudhuri K, Sugiyama M (eds) Proceedings of Machine Learning Research, Proceedings of Machine Learning Research, vol 89. PMLR, pp 3459–3467

Widmann D, Lindsten F, Zachariah D (2019) Calibration tests in multi-class classification: A unifying framework. In: NeurIPS

Zadrozny B, Elkan C (2002) Transforming classifier scores into accurate multi-class probability estimates. In: Proc. 8th Int. Conf. on Knowledge Discovery and Data Mining (KDD’02). ACM, pp 694–699

Zagoruyko S, Komodakis N (2016) Wide residual networks. CoRR abs/1605.07146. URL http://arxiv.org/abs/1605.07146, https://arxiv.org/abs/1605.07146

Zhang J, Kailkhura B, Han TY (2020) Mix-n-match: Ensemble and compositional methods for uncertainty calibration in deep learning. In: ICML
Contents

1 Introduction 1

2 Notation and Background 3
  2.1 True Calibration Error 3
  2.2 Reliability Diagrams and ECE 3
  2.3 Calibration Evaluation for Multi-Class 4
  2.4 Post-hoc Calibration 5

3 The Fit-on-the-Test Paradigm 6
  3.1 Fit-on-the-Test Calibration Evaluation 6
  3.2 Cross-Validated Number of Bins for ECE 8

4 Calibration Map Families PL and PL3 9
  4.1 PL - Piecewise Linear Calibration Maps 9
  4.2 PL3 - Piecewise Linear in Logit-Logit Space 11

5 Assessment of Calibrators and Evaluators 12
  5.1 Assessment of Post-hoc Calibrators 12
  5.2 Assessment of Calibration Evaluators 14

6 Experiments and Results 14

7 Conclusion and Future Work 17

A Source Code 22

B Proofs 22
  B.1 Definitions Related to Theorems 1 and 3 22
  B.2 Proof of Theorem 1 23
  B.3 Proof of Theorem 2 24
  B.4 Proof of Theorem 3 25

C Implementation Details 26
  C.1 Piecewise Linear Fitting Using a Neural Network 26
    C.1.1 PL Details 26
    C.1.2 PL3 Details 27
  C.2 Details of Cross-Validation 27
  C.3 Details About the Binning Methods 28
  C.4 Implementation Details of Other Methods 28
  C.5 Debiasing ECE 28

D Datasets and Experimental Setup 29
  D.1 List of Methods with Shortened Names 29
  D.2 Pseudo-Real Experiments 30
  D.3 Synthetic Experiments 30
D.4 Real Experiments .................................................. 31

E Visualizations of Calibration ...................................... 32
E.1 Comparisons of Reliability Diagrams ....................... 32
E.2 Calibration Maps in the Logit-Logit Scale ................. 34

F Results ................................................................ 34
F.1 Results of Pseudo-Real Experiments ......................... 34
   F.1.1 Results of Estimating the Reliability Diagram With $|\hat{c}_M - c^*|$ and $|\hat{c}_M - c^*|^2$ ......................... 35
   F.1.2 Results of Estimating the True Calibration Error with $|ECE_M - CE|$ and $|ECE_M - CE|^2$ .......... 36
F.2 Results of Synthetic Experiments .......................... 37
F.3 Results of Real Experiments ................................... 42
F.4 Running Time of the Experiments ............................ 44

G Limitations and Future Work .................................. 45

Appendix A Source Code

The source code is available at https://github.com/markus93/fit-on-the-test. It contains everything needed to run the experiments and to get the results displayed in the article. The source code contains a yml-file for generating a Conda environment with the needed packages and versions.

Appendix B Proofs

B.1 Definitions Related to Theorems 1 and 3

The main paper includes 3 theorems. Theorems 1 and 3 include Bregman divergences as a way to measure dissimilarity between two probability distributions. We use Bregman divergences in the context of binary class probability estimation, in which case a probability distribution can be represented by a single real number in the range $[0, 1]$, representing the probability for the positive class. Thus, in our case, Bregman divergences are functions that take in two positive class probabilities and output a real number representing the divergence of the distributions represented by these probabilities, $d : [0, 1] \times [0, 1] \to \mathbb{R}$. Note that the order of the two arguments is such that the first is the ‘prediction’ and the second is the ‘ground truth’ (we have seen both orders in the literature, but have found this order more natural). The formal definition is as follows:

**Definition 1** A function $d : [0, 1] \times [0, 1] \to \mathbb{R}$ is called a Bregman divergence, if there exists a continuously-differentiable and strictly convex function $\phi : [0, 1] \to \mathbb{R}$, such that for every $p, q \in [0, 1]$:

$$d(p, q) = \phi(q) - \phi(p) - (q - p)\phi'(p)$$

where $\phi'$ is the derivative of $\phi$. 
Theorems 1 and 3 involve random variables. As described in the main paper, we have \( X \) as a randomly drawn instance (i.e. \( X \) is a vector of its feature values) and \( Y \) is its label. In Theorem 1 we consider a particular fixed probabilistic classifier \( f : \mathcal{X} \rightarrow \mathbb{R} \) and thus, its output can be viewed as a random variable also, \( \hat{P} = f(X) \). The true calibration map of \( f \) can be calculated as \( c_f^*(\hat{p}) = \mathbb{E}[Y|f(X) = \hat{p}] = \mathbb{E}[Y|\hat{P} = \hat{p}] \) for any \( \hat{p} \in [0, 1] \).

In Theorem 3 we consider a particular calibrator \( \hat{c} : [0, 1] \rightarrow [0, 1] \), and the true calibration map of the approximately calibrated model \( \hat{c} \circ f \), which according to the definition of \( c^* \) can be written out as \( c_{\hat{c} \circ f}^*(c) = \mathbb{E}[Y|(\hat{c} \circ f)(X) = c] = \mathbb{E}[Y|\hat{c}(f(X)) = c] \) for any \( c \in [0, 1] \).

### B.2 Proof of Theorem 1

**Theorem 1** Let \( d : [0, 1] \times [0, 1] \rightarrow \mathbb{R} \) be any Bregman divergence and \( \hat{c}_1, \hat{c}_2 : [0, 1] \rightarrow [0, 1] \) be two estimated calibration maps. Then

\[
\mathbb{E}\left[d(\hat{c}_1(\hat{p}), Y) | \hat{P} = \hat{p}\right] - \mathbb{E}\left[d(\hat{c}_2(\hat{p}), Y) | \hat{P} = \hat{p}\right] = d\left(\hat{c}_1(\hat{p}), c_f^*(\hat{p})\right) - d\left(\hat{c}_2(\hat{p}), c_f^*(\hat{p})\right).
\]

**Proof** It is sufficient to prove that the value of the following expression does not depend on \( \hat{c}_i \) where \( i = 1 \) or \( i = 2 \) and thus is the same for \( \hat{c}_1 \) and \( \hat{c}_2 \):

\[
\mathbb{E}\left[d(\hat{c}_i(\hat{p}), Y) | \hat{P} = \hat{p}\right] - d\left(\hat{c}_i(\hat{p}), c_f^*(\hat{p})\right).
\]

Let \( \phi \) be a convex function that gives rise to \( d \), then according to the definition of the Bregman divergence we can rewrite the above expression as follows:

\[
\mathbb{E}\left[\phi(Y) - \phi(\hat{c}_i(\hat{p})) - (Y - \hat{c}_i(\hat{p}))\phi'(\hat{c}_i(\hat{p})) | \hat{P} = \hat{p}\right] - \left(\phi(c_f^*(\hat{p})) - \phi(\hat{c}_i(\hat{p})) - (c_f^*(\hat{p}) - \hat{c}_i(\hat{p}))\phi'(\hat{c}_i(\hat{p}))\right).
\]

As \( \mathbb{E}\left[\phi(Y) | \hat{P} = \hat{p}\right] \) and \( \phi(c_f^*(\hat{p})) \) do not depend on \( \hat{c}_i \) and as the terms \( \phi(\hat{c}_i(\hat{p})) \) and \( \hat{c}_i(\hat{p})\phi'(\hat{c}_i(\hat{p}))\) both cancel out, we are left to prove that the value of the remaining expression does not depend on \( \hat{c}_i \):

\[
\mathbb{E}\left[-Y\phi'(\hat{c}_i(\hat{p})) | \hat{P} = \hat{p}\right] + c_f^*(\hat{p})\phi'(\hat{c}_i(\hat{p})).
\]

Noting that \( \phi'(\hat{c}_i(\hat{p})) \) does not depend on \( \hat{P} \), it can be taken out from the expectation, and thus the expression can be written as:

\[
\left(-\mathbb{E}[Y | \hat{P} = \hat{p}] + c_f^*(\hat{p})\right)\phi'(\hat{c}_i(\hat{p})).
\]

However, this is equal to zero, since by the definition of the true calibration map \( c_f^* \) we have:

\[
c_f^*(\hat{p}) = \mathbb{E}[Y | \hat{P} = \hat{p}].
\]

\( \square \)
B.3 Proof of Theorem 2

Theorem 2 Consider a predictive model with predictions $\hat{p}_1, \ldots, \hat{p}_n \in [0, 1]$ on a

test set with actual labels $y_1, \ldots, y_n$ and a binning $B$ with $b \geq 1$ bins and boundaries

$0 = B_1 < \cdots < B_{b+1} = 1 + \epsilon$. Then for any $\alpha > 0$, the measure $ECE_B(\alpha)$ is equal to:

$$ECE_B(\alpha) = \frac{1}{n} \sum_{i=1}^{n} |\hat{c}(\hat{p}_i) - \hat{p}_i|^\alpha$$

where $\hat{c} = \arg \min_{C(B, H, 1)} \frac{1}{n} \sum_{i=1}^{n} (c(\hat{p}_i) - y_i)^2$

Furthermore, $\hat{c}(\bar{p}_k) = \bar{y}_k$ for $k = 1, \ldots, b$, where $\bar{p}_k$ and $\bar{y}_k$ are the average $\hat{p}_i$ and $y_i$ in the bin $[B_k, B_{k+1})$.

Proof Our first goal is to prove that $\hat{c}(\bar{p}_k) = \bar{y}_k$ for $k = 1, \ldots, b$. To find the values of

parameters at the optimum $\hat{c}$, we study the stated minimization task and consider any

c $\in C(B, H, 1)$ with any values of parameters $(H_1, \ldots, H_b)$. Let us rewrite the quantity

to be minimized, grouping the instances by bins and using the definition of $c(\cdot)$:

$$\frac{1}{n} \sum_{i=1}^{n} (c(\hat{p}_i) - y_i)^2$$

$$= \frac{1}{n} \sum_{k=1}^{b} \sum_{\hat{p}_i \in [B_k, B_{k+1})} (c(\hat{p}_i) - y_i)^2$$

$$= \frac{1}{n} \sum_{k=1}^{b} \sum_{\hat{p}_i \in [B_k, B_{k+1})} ((H_k + 1(\hat{p}_i - B_k)) - y_i)^2$$

Equating the derivatives of this expression with respect to each $H_k$ to zero, we get:

$$\frac{1}{n} \sum_{\hat{p}_i \in [B_k, B_{k+1})} 2(H_k + \hat{p}_i - B_k - y_i) = 0$$

$$\frac{2}{n} n_k (H_k - B_k) = \frac{2}{n} \sum_{\hat{p}_i \in [B_k, B_{k+1})} (y_i - \hat{p}_i)$$

$$H_k - B_k = \frac{1}{n_k} \sum_{\hat{p}_i \in [B_k, B_{k+1})} (y_i - \hat{p}_i)$$

$$H_k - B_k = \bar{y}_k - \bar{p}_k$$

for each $k$. Therefore, $H_k - B_k = \bar{y}_k - \bar{p}_k$ holds for the optimum at $\hat{c}$ and we get

$$\hat{c}(\bar{p}_k) = H_k + 1(\bar{p}_k - B_k) = \bar{p}_k + (H_k - B_k)$$

$$= \bar{p}_k + (\bar{y}_k - \bar{p}_k) = \bar{y}_k$$
More generally, for any \( \hat{p} \in [B_k, B_{k+1}) \) we get \( \hat{c}(\hat{p}) = H_{k+1}(\hat{p} - B_k) = \hat{p} + (H_k - B_k) = \hat{p} + (\bar{y}_k - \hat{y}_k) \). This implies that the term \( |\bar{p}_k - \hat{y}_k| \) in the definition of \( \text{CEAC} \) is equal to \( |\hat{c}(\hat{p}) - \hat{p}| \) for any \( \hat{p} \in [B_k, B_{k+1}) \). Using this, we can rewrite \( \text{ECE}^{(\alpha)} \) as follows:

\[
\text{ECE}^{(\alpha)}_B = \frac{1}{n} \sum_{k=1}^{b} n_k \cdot |\bar{p}_k - \bar{y}_k|^\alpha
\]

\[
= \frac{1}{n} \sum_{k=1}^{b} \sum_{\hat{p}_i \in [B_k, B_{k+1})} |\bar{p}_k - \bar{y}_k|^\alpha
\]

\[
= \frac{1}{n} \sum_{k=1}^{b} \sum_{\hat{p}_i \in [B_k, B_{k+1})} |\hat{c}(\hat{p}_i) - \hat{p}_i|^\alpha
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} |\hat{c}(\hat{p}_i) - \hat{p}_i|^\alpha
\]

\[\square\]

**B.4 Proof of Theorem 3**

Theorem 3 applies for any positive class probability estimator \( f : \mathcal{X} \to [0, 1] \), any calibrator \( \hat{c} : [0, 1] \to [0, 1] \), and any Bregman divergence \( d \). First we remind of the definitions of \( \text{CMEE} \) and \( \text{CEAC} \) given in the main paper:

- **Calibration error after calibration**: \( \text{CEAC} = \text{CE}(\hat{c} \circ f) = \mathbb{E}[d(\hat{C}, c^*_f(\hat{C}))] \)
- **Calibration map estimation error**: \( \text{CMEE} = \mathbb{E}[d(\hat{c}(\hat{P}), c^*_f(\hat{P}))] \)

where \( \hat{C} = \hat{c}(\hat{P}) = (\hat{c} \circ f)(X) = \hat{c}(f(X)) \).

**Theorem 3** \( \text{CMEE} = \text{CEAC} + \mathbb{E}[d(c^*_f(\hat{C}), c^*_f(\hat{P}))] \).

**Proof** We have to prove that \( \text{CEAC} + \mathbb{E}[d(c^*_f(\hat{C}), c^*_f(\hat{P}))] - \text{CMEE} = 0 \), that is:

\[
\mathbb{E}[d(\hat{C}, c^*_f(\hat{C}))] + \mathbb{E}[d(c^*_f(\hat{C}), c^*_f(\hat{P}))] - \mathbb{E}[d(\hat{C}, c^*_f(\hat{P}))] = 0.
\]

We will prove the variant of this equality where all expectations are replaced by conditional expectations conditioned on \( \hat{C} \), from which the original equality follows due to the law of total expectation, i.e. \( \mathbb{E}[\mathbb{E}[V|W]] = \mathbb{E}[V] \) for any random variables \( V \) and \( W \). That is, it is sufficient to prove that:

\[
\mathbb{E}\left[ d(\hat{C}, c^*_f(\hat{C})) \bigg| \hat{C} \right] + \mathbb{E}\left[ d(c^*_f(\hat{C}), c^*_f(\hat{P})) \bigg| \hat{C} \right] - \mathbb{E}\left[ d(\hat{C}, c^*_f(\hat{P})) \bigg| \hat{C} \right] = 0.
\]

Let \( \phi \) be a convex function that gives rise to \( d \), then according to the definition of the Bregman divergence we can rewrite the above equality as follows:

\[
\mathbb{E}\left[ \phi(c^*_f(\hat{C})) - \phi(\hat{C}) - (c^*_f(\hat{C}) - \hat{C})\phi'(\hat{C}) \bigg| \hat{C} \right] = 0.
\]
The first two terms in each conditional expectation cancel out among the three conditional expectations, leaving us with only the last terms. Taking into account that \( c_f^*(\hat{P}) \) is the only term which is not a constant under conditioning with \( \hat{C} \), the above is equivalent to:

\[
-((c_{\hat{c}_{\hat{C}}}^*(\hat{C})) - \hat{C})\phi'(\hat{C})
-((\mathbb{E}[c_f^*(\hat{P})|\hat{C}] - c_{\hat{c}_{\hat{C}}}^*(\hat{C}))\phi'(c_{\hat{c}_{\hat{C}}}^*(\hat{C}))
+(\mathbb{E}[c_f^*(\hat{P})|\hat{C}] - \hat{C})\phi'(\hat{C}) = 0.
\]

As \( \hat{C}\phi'(\hat{C}) \) cancels out, we can reorganise the remaining terms as follows:

\[
\left(\mathbb{E}[c_f^*(\hat{P})|\hat{C}] - c_{\hat{c}_{\hat{C}}}^*(\hat{C})\right)\left(\phi'(\hat{C}) - \phi'(c_{\hat{c}_{\hat{C}}}^*(\hat{C}))\right) = 0.
\]

It now suffices to prove that \( \mathbb{E}[c_f^*(\hat{P})|\hat{C}] = c_{\hat{c}_{\hat{C}}}^*(\hat{C}) \) for every value of \( \hat{C} \). According to the definition of the true calibration maps \( c_f^*(\hat{P}) \) and \( c_{\hat{c}_{\hat{C}}}^*(\hat{C}) \), this equality can be rewritten as:

\[
\mathbb{E}\left[\mathbb{E}[Y|\hat{P}]|\hat{C}\right] = \mathbb{E}[Y|\hat{C}].
\]

Since \( \hat{P} \) functionally determines \( \hat{C} \) through \( \hat{C} = \hat{c}(\hat{P}) \), the above equality follows directly from the law of total expectation applied on conditional expectations, i.e. \( \mathbb{E}\mathbb{E}[V|\mathcal{G}_2]|\mathcal{G}_1] = \mathbb{E}[V|\mathcal{G}_1] \) for any random variable \( V \) and \( \sigma \)-algebras \( \mathcal{G}_1 \subseteq \mathcal{G}_2 \). \( \square \)

## Appendix C  Implementation Details

This section provides the implementation details for all the methods used in the experiments.

### C.1  Piecewise Linear Fitting Using a Neural Network

#### C.1.1  PL Details

This section gives a more precise overview of implementation details of the piecewise linear method. Information about the overall architecture is available in the main part of the article. Furthermore, the exact implementation is available in the source code in the file "piecewise_linear.py".

The model is initialised such that it represents the identity calibration map. It is trained up to 1500 epochs. Early stopping patience is set to 20, which means that if the training loss has not gone smaller for 20 epochs, then the fitting is stopped. The model is optimized using Adam (Kingma and Ba, 2014) optimiser with the learning rate of 0.01. The batch size is \( \max(n_{\text{data}}/4, 512) \), e.g. for 1000 data points the batch size is 250, and for 10000 data points it is 512. Cross-validation is used to pick the number of nodes for the binning layer. The number of nodes minus 1 gives the number of bins. All numbers of bins from 1 bin to 16 bins are considered for the model. The only exception is when there are 1000 instances, where the maximum number of bins considered is 6. The model is trained using the MSE or cross-entropy loss. Cross-entropy
loss (CE) was showcased in the main article, due to better performance. In the following tables of results, $PL^{CE}_{NN}$ stands for training with the CE loss.

The $PL$ method fitting for a single model takes under 15 seconds, and with 10-fold cross-validation it takes up to 150 seconds depending on the number of nodes the model has. In total, finding the best number of bins (1 to 16 bins) with 10-fold CV takes up to 25 minutes depending on the data size and complexity of the fitted function. Mostly the model performs much faster, but it gets slower as more bins are used or the data sizes get bigger. Further speedups can be obtained by reducing the number of folds and the different numbers of bins considered in hyperparameter optimisation. The scripts were run in a high performance computing center using CPU processing power (Intel(R) Xeon(R) CPU E5-2660 v2 @ 2.20GHz) with up to 6GB of RAM.

C.1.2 PL3 Details

This section gives a further implementation details of the piecewise linear method in the logit-logit space. Similarly to PL, information about the overall architecture is available in the main part of the article and the exact implementation is available in source code in "piecewise_linear.py".

The model training part is exactly the same as for the PL method.

The PL3 method fitting tends to take more time comparing to PL method. Fitting a single model takes under 30 seconds, and with 10-fold cross-validation it takes up to 300 seconds. In total, finding the best number of bins with 10-fold CV takes up to 80 minutes. Large speedup can be obtained by reducing the number of folds and the different numbers of bins considered in hyperparameter optimisation.

C.2 Details of Cross-Validation

In our experiments, cross-validation is used to find the best number of bins for the $ES_{CV}$, $PL$ and $PL3$ methods. We have seen that the results improve by using a simple complexity-reducing regularisation trick, according to which we prefer a lower number of bins instead of a higher number of bins whenever the relative difference in the cross-validated loss estimate is less than 0.1 percent. Furthermore, the same way as in hyperparameter optimization for Dirichlet calibration (Kull et al, 2019), the predictions on test data are obtained as an average output from all the 10 models with the chosen number of segments but trained from different folds, i.e. we are not refitting a single model on all 10 folds.

Table F16 depicts the difference in results for estimating $|\hat{c}_M - c^*|$ with the classical CV and with the CV using the complexity-reducing regularisation. In Table F17 the same is depicted for estimating $|ECE_M - CE|$. It can be seen that the complexity reducing regularisation makes results better for $|\hat{c}_M - c^*|$ estimation in most cases. The only exception is $PL3^{CE}$, where the regularisation makes the results a tiny bit worse. On the other hand, the regularisation results
C.3 Details About the Binning Methods

The binning methods were implemented using NumPy and Scikit-Learn packages. The binning methods follow the approaches previously established, however cross-validation and unit-slope calibration maps are added. We have also implemented the sweep method to choose the highest number of bins just before the calibration map gets non-monotonic. All of the binning methods enable using both equal size and equal width binning. The implementation is available in the source code in the file "binnings.py".

C.4 Implementation Details of Other Methods

Other methods used for comparisons are taken from publicly available packages as follows: isotonic calibration and Platt scaling are available from the pycalib package (Nieto et al, 2019); beta calibration from the betacal package (Kull et al, 2017); KCE from the pycalibration package (Widmann et al, 2019) and \( PL_{DE} \) from the pwlf package (Jekel and Venter, 2019). For KCE we used the unbiased version with RBFKernel. Both, splines (Gupta et al, 2021) and intra-order preserving (IOP) functions (Rahimi et al, 2020) are implemented using official implementation provided in the original articles. The best number of splines for spline methods was found using CV similarly as for piecewise linear methods (Subsection C.2). For spline, three different methods were used: natural, parabolic and cubic. For IOP functions, the configurations given with original paper were used and two different versions: order-invariant (\( IOP_{OI} \)) and order-preserving (\( IOP_{OP} \)). Unfortunately, the third version, diagonal version, did not work. For KDE we used the implementation provided in the original article (Zhang et al, 2020). We used point-wise estimates for KDE as they seemed to offer better results than the integral based estimates proposed in the original article.

The best number of bins for \( PL_{DE} \) was found using CV similarly as for piecewise linear methods (Subsection C.2). The pwlf package also supports fitting piecewise quadratic curves (degree 2) in addition to the piecewise linear curves (degree 1). The degree 1 had better results than degree 2 according to the results in Table F12. For degree of 1, seven bins were chosen as the maximum limit for CV, as from there on the model fitting got very slow. For the degree of 2, five bins were chosen as the maximum limit for CV. On average, fitting \( PL_{DE} \) with 10-fold CV took about 30 minutes. The licenses of packages have been checked to be freely usable for our work.

C.5 Debiasing ECE

Debiasing was applied for the binning-based ECE methods. Reminding the notation, \( \bar{y}_k = \frac{1}{n_k} \sum_{\bar{p}_i \in [B_k, B_{k+1})} y_i \) is the average label in \( k \)-th bin, \( \bar{p}_k = \)
\[ \frac{1}{n_k} \sum_{\hat{p}_i \in [B_k, B_{k+1})} \hat{p}_i \] is the average prediction in \( k \)-th bin, \( n_k = |\{i \mid \hat{p}_i \in [B_k, B_{k+1})\}| \) is the size of bin \( k \), \( \text{ECE}^{(1)} \) is defined as \( \text{ECE}^{(1)}_B = \frac{1}{n} \sum_{k=1}^{b} n_k \cdot |\bar{p}_k - \bar{y}_k| \).

Kumar et al (2019) proposed to debias \( \text{ECE}^{(1)} \) by defining \( \bar{y}_k \) in each bin as a sample from a random variable defined by a Gaussian distribution \( N(\bar{y}_k, \bar{y}_k(1-\bar{y}_k) \frac{n_k}{n}) \). Bias can then be estimated by drawing repeated samples from the same random variable. The final debiased estimate of \( \text{CE}^{(1)} \) can then be achieved by subtracting the approximated bias from the \( \text{ECE}^{(1)} \) value.

Instead of drawing repeated random samples, we propose to use integration and the probability density function of the same random variable for computationally faster results. Instead of drawing samples from \( R_k \sim N(\bar{y}_k, \bar{y}_k(1-\bar{y}_k) \frac{n_k}{n}) \) for each bin to find \( \mathbb{E}[n_k \cdot |\bar{p}_k - R_k|] \) as proposed by Kumar et al (2019), one can find it computationally faster by finding in each bin

\[ \int_{-\infty}^{\infty} n_k \cdot |\bar{p}_k - x| \cdot f_{R_k}(x) \, dx, \]

where \( f_{R_k} \) is the probability density function of \( R_k \). We used the simple trapezoidal integration with 10k equally-spaced integration points within the area up to 5 standard deviations away from the mean.

Appendix D Datasets and Experimental Setup

We ran experiments on pseudo-real, synthetic and real datasets. More details about these datasets and the experimental setup is in the following sections. We have checked the licenses of datasets and confirmed that these datasets are freely usable for this work.

D.1 List of Methods with Shortened Names

- \( ES_{15} \) - ECE method with equal-size binning and 15 bins, \( EW \) for equal-width binning;
- \( ES_{\text{sweep}} \) - ECE method with equal-size binning and sweep method for choosing the number of bins;
- \( ES_{\text{CV}} \) - ECE method with equal-size binning and cross-validation for choosing the number of bins;
- Platt - platt scaling;
- beta - Beta calibration;
- isotonic - isotonic calibration;
- Scaling-Binning - scaling-binning method;
- TempS/VecS - temperature/vector scaling;
- MSODIR - matrix scaling with off-diagonal and intercept regularisation;
- dirODIR/dirL2 - dirichlet calibration with ODIR and L2 regularisation;
- 1-Temp - temperature scaling learning in 1-vs-rest fashion;
• Spline (natural/cubic/parabolic) - spline calibration with different methods;
• \( IOP_{OI} \) and \( IOP_{OP} \) - intra-order preserving functions with order-invariant and order-preserving variants;
• \( PL_{CE}^{NN} \) and \( PL_{MSE}^{NN} \) - piecewise linear method with cross-entropy or MSE loss;
• \( PL^{CE}_3 \) - piecewise linear method in logit-logit space;
• \( PL_{DE} \) - piecewise linear method based on least squares fitting with differential evolution. \( PL_{DE}^{2} \) - degree 2 for quadratic curves;
• KDE - kernel density estimation;
• KCE - kernel calibration error.

D.2 Pseudo-Real Experiments

The pseudo-real dataset is called CIFAR-5m (Nakkiran et al, 2021) and contains over 5 million synthetic images similar to CIFAR-10 (Krizhevsky et al, 2009) with size of 32x32 pixels. These images were created by sampling DDPM model (Ho et al, 2020) trained on CIFAR-10 data. The pseudo-real data was used to get close to real data with the advantage of being able to estimate the true calibration map very precisely.

In order to estimate the true calibration map on 1 million hold-out data-points 3 different calibration methods were used: (1) isotonic calibration; (2) equal size binning with 100 bins with flat-top (i.e. slope 0) bins; (3) equal size binning with 100 bins with slope-1-tops (i.e. tops of the bins parallel to the main diagonal). Only minor differences across different ‘true’ calibration maps occurred (see Tables F2, F6 and F7).

To set up the experiments, the datasets were calibrated with various 2-class calibration methods (beta, isotonic, Platt, 1-Temp, ScalingBinning), multiclass calibrators (TempS, VecS, MSODIR, dirL2, dirODIR, IOP, Spline), piecewise linear methods \( PL_3 \), \( PL_{NN} \) with cross-entropy loss, and the method \( ES_{sweep} \) adapted from calibration evaluation to calibration map fitting. Table F1 compares the results. The calibration is done in 1-vs-Rest fashion to achieve results for a 2-class problem. We have 1 confidence calibration task and 3 one-vs-Rest subtasks (car, cat, dog), for 6 calibration methods on 3 models, in total 72 combinations. The 6 calibration methods were chosen as the best methods in Table 1 of the main article: beta, vector scaling, Platt, PL3, ScalingBinning, isotonic.

D.3 Synthetic Experiments

For synthetic data, only the predicted probabilities \( \hat{p} \), labels \( y \), and corresponding calibrated probabilities \( c^*_f(\hat{p}) \) were generated. Synthetic data were generated based on five different base shapes (Figure D1). The 4 first shapes were chosen to mimic likely scenarios of calibration mappings, with combinations of over- and under-confidence for values below and above 0.5. The 5th shape ‘stairs’ was added as a more challenging shape that crosses the identity function in two places.
From each shape, multiple variants that we refer to as 'derivates' were generated by linearly mixing the shape with the identity function in different proportions. Derivates were generated to have datasets with different expected calibration errors. To generate a synthetic dataset from a particular derivate, first the calibrated probabilities $c^*_f(\hat{p})$ were sampled from a base distribution. Then the labels $y$ were sampled from the calibrated probabilities. Finally, the derivate was used to transform the calibrated probabilities $c^*_f(\hat{p})$ to their corresponding predicted probabilities $\hat{p}$. Therefore, the construction of derivates creates the inverse of the calibration map, and then the calibration map can be obtained from it by inverting the function. It might seem more intuitive to first sample the predicted probabilities $\hat{p}$ and then use the true calibration map to find the corresponding calibrated probabilities $c^*_f(\hat{p})$. However, the more unintuitive approach used here has the following benefit the other approach does not. Namely, by first sampling $c^*_f(\hat{p})$ and the labels, we can generate synthetic datasets that have the exact same set of labels but different predicted probabilities. This allows to mimic a realistic scenario where we have several models trained on the same dataset and we would like to choose the model with the lowest calibration error. E.g., if we would like to rank different post-hoc calibration methods. This fact has been used to generate Table F23. The five base shapes were defined by the following functions from $c^*_f(\hat{p})$ to $\hat{p}$:

- $\text{square}(x) = x^2$
- $\text{sqrt}(x) = \sqrt{x}$
- $\text{beta1}(x) = 1/(1 + 1/(e^c \cdot x^a/(1 - x)^b))$
  where $a = 0.4, b = 0.45, c = b \ln(0.6) - a \ln(0.4)$
- $\text{beta2}(x) = 1/(1 + 1/(e^c \cdot x^a/(1 - x)^b))$
  where $a = 2, b = 2.2, c = b \ln(0.52) - a \ln(0.48)$
- $\text{stairs}(x) = \text{stairs}_\text{helper}(x + 1/3) - \text{stairs}_\text{helper}(1/3)$
  where $\text{stairs}_\text{helper}(x) = \text{step}(\text{step}(3x\pi))/(3\pi)$, and $\text{step}(x) = x - \sin(x)$

Synthetic data were generated for data sizes 1000, 3000, 10000 with 5 different data seeds. The calibrated predictions $c^*_f(\hat{p})$ were sampled from the uniform distribution. Derivates with expected absolute calibration errors 0.00, 0.005, 0.01, ..., 0.10 were generated for each of the 5 base shapes. In total, we used 3 data sizes, 5 random seeds, 5 base shapes, and 21 derivates per shape. In Figure D1, two examples of derivates for the "stairs" function are also shown. Note that the derivates have been obtained by linear mixing with the identity function in the horizontal direction because of creating the inverse calibration maps first.

For Figure 1 and Figure 2 in the main article 3000 data points were generated in the way described above. Uniform distribution and the base function $\text{beta2}$ were used.

### D.4 Real Experiments

The real dataset contains 60k images from CIFAR-10/100 (Krizhevsky et al., 2009) with size of 32x32 pixels with 10 or 100 classes. Each of the datasets
Fig. D1: Base shapes used for generating synthetic data. The last plot also contains two examples of derivates with expected absolute calibration errors 0.03 and 0.07 for the Uniform distribution.

Fig. E2: Reliability diagrams on synthetic data. 10k datapoints. Derivate with 0.10 expected absolute calibration error for square.

have 5k validation and 10k train instances. In total, there are 10 model-dataset combinations, the model outputs have been calibrated using 5 different methods (TempS (Guo et al, 2017), VecS (Guo et al, 2017), MS_ODIR (Guo et al, 2017), dir_L2 (Kull et al, 2019), dir_ODIR (Kull et al, 2019)) using the validation set. This gives us 50 datasets of model and calibration method combinations. To have a comparison with the synthetic data, we extracted test data subsets of sizes 1000 (10 sets), 3000 (3 sets), 10000 (1 set). The number of sets is also multiplied by 5, as there were 5 different calibration methods. In total, we got 500 sets with 1000 instances, 150 sets with 3000 instances, and 50 sets with 10000 instances.

Appendix E  Visualizations of Calibration

E.1 Comparisons of Reliability Diagrams

Figures E2-E6 depict comparisons between different reliability diagrams obtained on synthetic data with 10000 instances, true calibration error 0.1 and different calibration functions. The middle three diagrams of every figure are depicted with slope 1 (CE estimation by fitting). Therefore, the diagrams for ES_sweep might not seem monotonic, but they would be if they were plotted with the classic flat bin roofs. Based on the figures, the piecewise linear method is able to follow the true calibration map the best.
Fig. E3: Reliability diagrams on synthetic data. 10k datapoints. Derivate with 0.10 expected absolute calibration error for $sqrt$.

Fig. E4: Reliability diagrams on synthetic data. 10k datapoints. Derivate with 0.10 expected absolute calibration error for $beta1$.

Fig. E5: Reliability diagrams on synthetic data. 10k datapoints. Derivate with 0.10 expected absolute calibration error for $beta2$.

Fig. E6: Reliability diagrams on synthetic data. 10k datapoints. Derivate with 0.10 expected absolute calibration error for $stairs$. 
E.2 Calibration Maps in the Logit-Logit Scale

As proved in the main paper, the temperature scaling method applied in binary classification fits a calibration map which is linear in the logit-logit scale. Furthermore, here we show that the beta calibration method fits a calibration map which is approximately piecewise linear in the logit-logit scale with 2 pieces.

Consider the calibration map family of beta calibration, \( \hat{c}(\hat{p}) = \frac{1}{1+1/(e^{c\hat{p}^a/(1-\hat{p})^b})} \). Changing the y-axis to logit scale, we get

\[
\ln\left(\frac{\hat{c}(\hat{p})}{1-\hat{c}(\hat{p})}\right) = \ln\left(e^{c\hat{p}^a/(1-\hat{p})^b}\right) = c + a \ln\hat{p} - b \ln(1-\hat{p}).
\]

We can rewrite it in two ways:

\[
\ln\left(\frac{\hat{c}(\hat{p})}{1-\hat{c}(\hat{p})}\right) = c + a \ln\left(\frac{\hat{p}}{1-\hat{p}}\right) + (a-b) \ln(1-\hat{p})
\]
\[
\ln\left(\frac{\hat{c}(\hat{p})}{1-\hat{c}(\hat{p})}\right) = c + b \ln\left(\frac{\hat{p}}{1-\hat{p}}\right) + (a-b) \ln\hat{p}.
\]

For low values of \( \hat{p} \) near 0, the term \((a-b) \ln(1-\hat{p})\) in the first way of writing is nearly zero, and thus we get a linear approximation in the logit-logit scale with slope \( a \). For high values of \( \hat{p} \) near 1, the term \((a-b) \ln\hat{p}\) in the second way of writing is nearly zero, and thus we get a linear approximation in the logit-logit scale with slope \( b \). This can be clearly seen visually in Figure E7, where the breakpoint between the two pieces is at \( \hat{p} = 0.5 \) and near this point the two linear segments are interpolated non-linearly.

Figure 4a from the main article shows a case from the pseudo-real dataset. As seen in the figure on the right, PL3 has been able to approximate most of the true calibration map quite well in the logit-logit space piecewise linearly, with two long linear segments (and a third short segment to the right of \( 1 - 10^{-6} \)). In contrast, beta calibration has failed to capture these segments because it is bound to have the breakpoint between the two segments at \( \hat{p} = 0.5 \).

Appendix F Results

F.1 Results of Pseudo-Real Experiments

Here is a brief guide to how we have arranged the tables with the results:

- Table F1. Pseudo-Real: Calibration method comparison;
- Tables F2 and F3. Pseudo-Real: Calibration Maps - absolute and square errors;
- Tables F4 and F5. Pseudo-Real: ECE - absolute and square errors;
- Tables F6, F7, F8 and F9. Pseudo-Real: Different ground-truths;
Fig. E7: Left: beta calibration map with parameters $(a = 0.3; b = 1.4; c = 0.0)$; Right: the same calibration map in the logit-logit space, illustrating that beta calibration approximately fits a piecewise linear calibration map with 2 segments.

Table F1: $PL$-methods, binning methods and various other calibration methods used for calibration. Evaluated on CIFAR-5m. The table displays thousandths of $|\hat{c}_M - c^*|$. The value of $c^*$ was found by estimating the true calibration map on $10^6$ unseen data with isotonic regression.

| Method | Cal. Bic. | $PL_{DE}$ | $PL_{SL}$ | $PL_{SL}^{cDE}$ | $PL_{SL}^{cDE}$ | $PL_{DE}$ | $PL_{SL}$ | $PL_{SL}^{cDE}$ | $PL_{SL}^{cDE}$ | $PL_{DE}$ | $PL_{SL}$ | $PL_{SL}^{cDE}$ | $PL_{SL}^{cDE}$ |
|--------|-----------|-----------|-----------|-----------------|-----------------|-----------|-----------|-----------------|-----------------|-----------|-----------|-----------------|-----------------|
| Platt  |   0.00    |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |
| Beta   |   0.00    |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |
| IsotonicRegression |   0.00    |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |
| IOP    |   0.00    |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |
| MSE    |   0.00    |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |
| NN     |   0.00    |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |   0.00    |   0.00    |     0.00        |     0.00        |

- Tables F10 and F11. Pseudo-Real: Comparison of different numbers of instances;
- Tables F12 and F13. Pseudo-Real: CE and MSE comparison, including $PL_{DE}$ with degree 1 and 2;
- Tables F14 and F15. Pseudo-Real: Equal-size vs equal-width;
- Tables F16 and F17. Pseudo-Real: CV Regularisation;
- Tables F18 and F19. Pseudo-Real: Standard Deviations;
- Tables F20, F21, F22 and F23. Synthetic: results;
- Table F24. Real: biases.

### F.1.1 Results of Estimating the Reliability Diagram With $|\hat{c}_M - c^*|$ and $|\hat{c}_M - c^*|^2$

The following paragraphs have results of estimating the reliability diagram with $|\hat{c}_M - c^*|$ and $|\hat{c}_M - c^*|^2$ on CIFAR-5m.

Results on CIFAR-5m indicate that the performance for measures vary over different methods. However, beta calibration and piecewise linear methods PL and PL3 with cross-entropy loss are in the lead. Beta calibration has average rank of 4.6, $PL_{DE}^{CE}$ has average rank of 4.2, $PL_{NN}^{MSE}$ has average rank of 3.4
and $PL_{NN}^{CE}$ has average rank of 1.2 (Table F2). In case of quadratic loss, $PL_{NN}^{CE}$ and $PL_{NN}^{MSE}$ perform the best, followed by $IOP_{OI}$, $PL_{NN}^{3CE}$, $ES_{10}$ and beta calibration (Table F3). Note that $PL_{NN}^{MSE}$ performs well, however it is clearly outperformed by $PL_{NN}^{CE}$.

The number of data instances (Table F10), does not change much the overall ordering. However, the more data instances, the better all models are, at getting closer to true calibration map. Additionally, as stated in the main article, the beta calibration works really well with smaller data sizes - 1000, 3000, similarly $IOP_{OI}$.

Next, the cross-entropy loss seems to be beneficial for both $PL_{3}$ and $PL_{NN}$ methods (Table F12). The method $PL_{DE}$ with degree of 1 is performing better than with degree of 2. Overall, $PL_{DE}$ is mostly behind $PL_{3}$ and $PL_{NN}$ with CE loss.

As expected, equal-size (ES) binning methods performed much better than equal-width (EW) binning methods (Table F14). Furthermore, comparing $ES_{sweep}$ with $ES_{CV}$, CV variant gets better results 8 times out of 12 and thus getting also better average ranking 8.8 compared to average rank 11.3 of sweep (Table F2).

The standard deviations (Table F18) of calibration measures are really similar, only $PL_{DE}$ and $KDE$ perform worse than other methods. Interestingly, the standard deviations are generally higher for DenseNet40 with confidence dataset.

Different estimated ground-truths (isotonic; equal-size binning with flat tops; with slope 1 tops) of CIFAR-5m data, result in only minor differences (Tables F2, F6, F7).

F.1.2 Results of Estimating the True Calibration Error with $|ECE_{M} - CE|$ and $|ECE_{M} - CE|^2$

The following paragraphs have results of estimating the true calibration error with $|ECE_{M} - CE|$ and $|ECE_{M} - CE|^2$ on CIFAR-5m.

$ECE_{15}$ (among all ES) and $PL_{3}^{CE}$ are the best at estimating calibration error, with average ranks of 3.8 and 5.2 (Table F4). On the other hand, the best measures for the quadratic loss are $PL_{NN}^{CE}$ with the average rank of 2.8 and $IOP_{OI}$ with the average rank of 4.2 (Table F5).

The number of data instances (Table F11), does not change the ranking for most methods, similarly to estimating the true calibration map. In comparison between other methods, $ES_{sweep}$, $beta$, and $IOP_{OI}$ work better with less data, while $ES_{20}$, $ES_{25}$, $ES_{CV}$ work better with more data. Furthermore, again all the methods get more accurate with more data.

The cross-entropy loss is beneficial for $PL_{3}$, but $PL_{NN}$ with MSE loss is better at estimating $|ECE_{M} - CE|$ (Table F13). Again, $PL_{DE}$ with degree 1 is outperforming degree 2. $PL_{3}$ with CE loss is the best at estimating $|ECE_{M} - CE|$ among piecewise linear methods.

For estimating $|ECE_{M} - CE|$, equal-size binning methods performed much better than equal-width binning methods (Table F15), the only exception
Table F2: Comparison of calibration evaluators in estimating the reliability diagram with $| \hat{c}_M - c^* |$ on CIFAR-5m. The initial model predictions have been calibrated by 6 different methods on 5k data points. Corresponding methods (columns) have been then used to estimate the true calibration map on a new unseen test set of size 1k, 3k, 10k. Average of 5 test set data seeds. In total, a single cell value is the average of 6x3x5=90 calibration map estimates. The value of $c^*$ was found by estimating the true calibration map on $10^6$ unseen data with isotonic regression. The table displays thousandths.

| Model        | ES10 | ES20 | ES30 | ES40 | ES50 | ES60 | ES70 | ES80 | ES90 | SD10 | SD20 | SD30 | SD40 | SD50 | SD60 | SD70 | SD80 | SD90 | SC10 | SC20 | SC30 | SC40 | SC50 | SC60 | SC70 | SC80 | SC90 | SC100 | SC200 | SC300 | SC400 | SC500 | SC600 | SC700 | SC800 | SC900 | SC1000 | SC1500 |
|--------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|--------|
| ResNet-18    | 0.001| 0.002| 0.001| 0.001| 0.002| 0.002| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001 |
| DenseNet-40   | 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001 |
| Table F3: Comparison of calibration evaluators in estimating the reliability diagram with $| \hat{c}_M - c^* |^2$ on CIFAR-5m. Otherwise like Table F2.

| Model        | ES10 | ES20 | ES30 | ES40 | ES50 | ES60 | ES70 | ES80 | ES90 | SD10 | SD20 | SD30 | SD40 | SD50 | SD60 | SD70 | SD80 | SD90 | SD10 | SD20 | SD30 | SD40 | SD50 | SD60 | SD70 | SD80 | SD90 | SD100 | SD200 | SD300 | SD400 | SD500 | SD600 | SD700 | SD800 | SD900 | SD1000 | SD1500 |
|--------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|--------|
| ResNet-18    | 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001 |
| DenseNet-40   | 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001| 0.001 |

is $ES_{10}$, where equal-size performs similarly to equal-width binning. Next, comparing $ES_{sweep}$ with $ES_{CV}$, $ES_{sweep}$ is better at absolute error, however $ES_{CV}$ is better at quadratic error (Tables F4 and F5).

The standard deviations (Table F19) of calibration measures are really similar, only $PL_{DE}$ and $KDE$ perform worse than other methods.

Different estimated ground-truths (isotonic; equal-size binning with flat tops; with slope 1 tops) of CIFAR-5m data, result in only minor differences; however, it does change the top-1 ranking method (Tables F8, F9 and Table 3 from the main article).

F.2 Results of Synthetic Experiments

The results of synthetic experiments indicate that beta calibration and Platt scaling are very good when the parametric family is able to approximate $c^*$ closely (Table F20). However, these methods can fail for more difficult shapes (i.e. ‘stairs’). Piecwise linear methods are following in performance and the binning methods are in last place. To achieve a good score for all the shapes, the piecewise linear methods should be picked. The repeating results for isotonic in Table F20 are not a bug, but a peculiarity arising from the way synthetic data were generated.
Table F4: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_M - CE|$ on CIFAR-5m. Evaluated on CIFAR-5m. The initial model predictions have been calibrated by 6 different methods on 5k data points. Corresponding methods (columns) have been then used to estimate the true calibration map on a new unseen test set of size 1k, 3k, 10k. Average of 5 test set data seeds. In total, a single cell value is the average of 6x3x5=90 calibration map estimates. The value of c was found by estimating the true calibration map on $10^6$ unseen data with isotonic regression. The table displays thousands.

| Method    | c   | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  |
|-----------|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| Baseline  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Averaged  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LM        | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| MTL       | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

Table F5: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_M - CE|^2$ on CIFAR-5m. Otherwise like Table F4.

| Method    | c   | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  |
|-----------|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| Baseline  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Averaged  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LM        | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| MTL       | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

Table F6: Comparison of calibration evaluators in estimating the reliability diagram with $|\hat{c}_M - c^*|$ on CIFAR-5m. The value of $c^*$ was found by estimating the true calibration map on $10^6$ unseen data with equal size binning with 100 bins with slope 1 instead of isotonic regression. Otherwise like Table F2.

| Method    | c   | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  |
|-----------|-----|------|------|------|------|------|------|------|------|------|
| Baseline  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Averaged  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LM        | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| MTL       | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

Table F7: Comparison of calibration evaluators in estimating the reliability diagram with $|\hat{c}_M - c^*|$ on CIFAR-5m. The value of $c^*$ was found by estimating the true calibration map on $10^6$ unseen data with equal size binning with 100 bins with flat bin bin tops instead of isotonic regression. Otherwise like Table F2.

| Method    | c   | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  | 1k   | 3k   | 10k  |
|-----------|-----|------|------|------|------|------|------|------|------|------|
| Baseline  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Averaged  | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| LM        | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| MTL       | 0.00| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
Table F8: Comparison of calibration evaluators in estimating the true calibration error with \( |ECE_M - CE| \) (measured in thousandths) and the ranking of 6 calibrators (Spearman rankcorrel(\(ECE\))) on CIFAR-5m. The value of \( c \) was found by estimating the true calibration map on \( 10^6 \) unseen data with equal size binning with 100 bins with slope 1 instead of isotonic regression.

| Metric | Data | \( E_{50} \) | \( E_{50\text{non}} \) | \( E_{50\text{na}} \) | \( E_{50\text{CV}} \) | \( P_5 \) | \( PL_5 \) | Platt | data | isotonic | Spline | natural | ROI\(_{50}\) |
|------|------|-----------|-----------------|-----------------|-----------------|-----|-----|------|------|-------|-------|-------|-------|
| \( |ECE_M - CE| \) one-event confidence | 4.79 | 3.73 | 4.07 | 3.04 | 3.57 | 4.62 | 3.84 | 4.03 | 4.34 | 4.04 | 4.04 |
| \( \text{rankcorrel}(ECE) \) one-event confidence | 0.036 | 0.146 | 0.392 | 0.254 | 0.471 | 0.056 | 0.124 | 0.409 | 0.471 | -0.006 |

Table F9: Comparison of calibration evaluators in estimating the true calibration error with \( |ECE_M - CE| \) (measured in thousandths) and the ranking of 6 calibrators (Spearman rankcorrel(\(ECE\))) on CIFAR-5m. The value of \( c \) was found by estimating the true calibration map on \( 10^6 \) unseen data with equal size binning with 100 bins with flat bin tops instead of isotonic regression.

| Metric | Data | \( E_{50} \) | \( E_{50\text{non}} \) | \( E_{50\text{na}} \) | \( E_{50\text{CV}} \) | \( P_5 \) | \( PL_5 \) | Platt | data | isotonic | Spline | natural | ROI\(_{50}\) |
|------|------|-----------|-----------------|-----------------|-----------------|-----|-----|------|------|-------|-------|-------|-------|
| \( |ECE_M - CE| \) one-event confidence | 5.89 | 5.04 | 5.01 | 3.09 | 4.72 | 4.63 | 4.18 | 3.74 | 5.84 | 5.75 |
| \( \text{rankcorrel}(ECE) \) one-event confidence | 0.194 | 0.261 | 0.146 | 0.126 | 0.345 | 0.157 | 0.136 | 0.226 | 0.548 | 0.084 |

Table F10: Comparison of calibration evaluators in estimating the reliability diagram with \( |\hat{c}_M - c^*| \) on CIFAR-5m. Aggregate over different data sizes. In total, a single cell value is the average of 6x4x5=120 calibration map estimates, where 4 is number of 2 class problems (1vsRest and confidence). Otherwise like Table F2.

| Metric | Data | \( E_{50} \) | \( E_{50\text{non}} \) | \( E_{50\text{na}} \) | \( E_{50\text{CV}} \) | \( P_5 \) | \( PL_5 \) | Platt | data | isotonic | Spline | natural | ROI\(_{50}\) |
|------|------|-----------|-----------------|-----------------|-----------------|-----|-----|------|------|-------|-------|-------|-------|
| \( \text{rankcorrel}(ECE) \) one-event confidence | 0.194 | 0.261 | 0.146 | 0.126 | 0.345 | 0.157 | 0.136 | 0.226 | 0.548 | 0.084 |

Table F11: Comparison of calibration evaluators in estimating the true calibration error with \( |ECE_M - CE| \) on CIFAR-5m. Aggregate over different data sizes. In total, a single cell value is the average of 6x4x5=120 calibration map estimates, where 4 is number of 2 class problems (1vsRest and confidence). Otherwise like Table F4.
Table F12: Comparison of calibration evaluators in estimating the reliability diagram with $|\hat{c}_M - c^*|$ on CIFAR-5m. Table compares piecewise linear methods with MSE and cross-entropy loss and $PL_{DE}$ method with degree 1 and 2. Otherwise like Table F2.

| Model | binning | $PL^{CE}_{NN}$ | $PL^{MSE}_{NN}$ | $PL^{CE}_{DE}$ | $PL^{MSE}_{DE}$ | $PL_{DE}$ | $PL^2_{DE}$ |
|-------|---------|----------------|-----------------|----------------|-----------------|---------|-------------|
| resnet110 | cars vs rest | 3.52 | 4.57 | 3.18 | 3.64 | 3.92 | 3.77 |
| | cats vs rest | 7.72 | 9.75 | 7.44 | 8.33 | 10.17 | 9.47 |
| | dogs vs rest | 7.04 | 8.93 | 6.37 | 7.73 | 8.97 | 9.57 |
| | confidence | 11.09 | 11.63 | 9.79 | 10.84 | 11.76 | 11.66 |
| densenet40 | cars vs rest | 3.32 | 4.53 | 2.43 | 3.21 | 4.21 | 4.02 |
| | cats vs rest | 7.16 | 8.49 | 5.72 | 6.61 | 7.64 | 8.25 |
| | dogs vs rest | 6.79 | 7.66 | 5.02 | 6.17 | 6.94 | 6.95 |
| | confidence | 11.05 | 12.09 | 10.75 | 11.56 | 11.37 | 11.99 |
| wide32 | cars vs rest | 3.89 | 5.06 | 2.62 | 3.22 | 3.66 | 3.91 |
| | cats vs rest | 7.43 | 9.29 | 6.75 | 7.41 | 8.84 | 9.01 |
| | dogs vs rest | 8.19 | 9.41 | 6.01 | 6.89 | 8.53 | 8.43 |
| | confidence | 10.03 | 10.64 | 9.21 | 10.05 | 9.76 | 10.04 |
| avg rank | | 2.8 | 5.6 | 1.0 | 2.7 | 4.3 | 4.7 |

Table F13: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_M - CE|$ on CIFAR-5m. Table compares piecewise linear methods with MSE and cross-entropy loss and $PL_{DE}$ method with degree 1 and 2. Otherwise like Table F4.

| Model | binning | $PL^{CE}_{NN}$ | $PL^{MSE}_{NN}$ | $PL^{CE}_{DE}$ | $PL^{MSE}_{DE}$ | $PL_{DE}$ | $PL^2_{DE}$ |
|-------|---------|----------------|-----------------|----------------|-----------------|---------|-------------|
| resnet110 | cars vs rest | 1.36 | 2.15 | 2.03 | 1.71 | 1.83 | 2.04 |
| | cats vs rest | 2.58 | 4.08 | 3.65 | 3.17 | 3.29 | 3.33 |
| | dogs vs rest | 2.91 | 4.06 | 3.55 | 3.74 | 3.96 | 3.99 |
| | confidence | 4.02 | 4.56 | 4.39 | 4.72 | 4.29 | 4.52 |
| densenet40 | cars vs rest | 1.38 | 2.62 | 1.49 | 1.45 | 2.14 | 2.19 |
| | cats vs rest | 3.35 | 4.82 | 3.64 | 3.45 | 3.45 | 3.66 |
| | dogs vs rest | 3.29 | 4.48 | 2.83 | 2.43 | 2.92 | 2.47 |
| | confidence | 5.27 | 5.62 | 5.97 | 5.59 | 5.31 | 6.08 |
| wide32 | cars vs rest | 1.39 | 2.56 | 1.73 | 1.83 | 1.62 | 1.87 |
| | cats vs rest | 2.95 | 4.46 | 3.87 | 3.26 | 3.44 | 3.63 |
| | dogs vs rest | 4.04 | 5.26 | 3.12 | 3.23 | 4.23 | 4.18 |
| | confidence | 4.89 | 4.32 | 5.56 | 5.09 | 4.43 | 4.84 |
| avg rank | | 1.8 | 5.3 | 3.8 | 2.8 | 3.1 | 4.2 |

Performance of with regards to $|ECE_M - CE|$ is similar to $|\hat{c}_M - c^*|$ (Table F21). The best measure is $PL_{DE}$ and measures Platt scaling and ESCV are following. Again, Platt scaling and beta calibration are failing at ‘stairs’ dataset.

In Table F22 the performance of estimating $|ECE_M - CE|^2$ is compared so that KCE could also be included. The unbiased version of KCE with RBFKernel is used. KCE performs worse than the other selected methods.
### Table F14: Comparison of calibration evaluators in estimating the reliability diagram with $|\hat{c}_M - c^*|$ on CIFAR-5m. Table compares equal-size binning with equal-width binning. Otherwise like Table F2.

| Model      | binning | $EW_{10}$ | $ES_{10}$ | $EW_{15}$ | $ES_{15}$ | $EW_{20}$ | $ES_{20}$ | $EW_{CV}$ | $ES_{CV}$ |
|------------|---------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| resnet110  | cars vs rest | 4.775 | 4.384 | 5.137 | 3.782 | 5.418 | 3.711 | 4.946 | 3.943 |
|            | confidence | 11.284 | 8.941 | 12.037 | 10.431 | 12.748 | 10.772 | 11.495 | 10.042 |
| densenet40 | cars vs rest | 4.673 | 7.849 | 4.995 | 4.964 | 5.257 | 5.156 | 4.623 | 3.791 |
|            | confidence | 10.284 | 10.044 | 11.436 | 11.937 | 12.698 | 9.613 | 8.452 | 9.212 |
| wide32     | cars vs rest | 4.536 | 3.753 | 5.089 | 3.481 | 5.618 | 3.652 | 3.995 | 3.764 |
|            | confidence | 10.426 | 9.944 | 11.449 | 9.012 | 12.628 | 10.092 | 9.583 | 8.571 |

 avg rank: 4.9 2.6 6.6 3.5 7.9 4.6 3.8 2.1

### Table F15: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_M - CE|$ on CIFAR-5m. Table compares equal-size binning with equal-width binning. Otherwise like Table F4.

| Model      | binning | $EW_{10}$ | $ES_{10}$ | $EW_{15}$ | $ES_{15}$ | $EW_{20}$ | $ES_{20}$ | $EW_{CV}$ | $ES_{CV}$ |
|------------|---------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| resnet110  | cars vs rest | 1.461 | 1.996 | 1.462 | 1.855 | 1.634 | 1.854 | 2.868 | 2.847 |
|            | cats vs rest | 2.816 | 2.321 | 2.755 | 2.352 | 2.754 | 2.373 | 4.093 | 3.167 |
|            | dogs vs rest | 2.983 | 3.294 | 3.406 | 2.831 | 3.475 | 2.882 | 4.047 | 4.248 |
|            | confidence | 4.021 | 4.163 | 4.052 | 4.451 | 4.261 | 4.295 | 7.185 | 6.687 |
| densenet40 | cars vs rest | 1.464 | 1.232 | 1.505 | 1.111 | 1.724 | 1.287 | 2.978 | 2.317 |
|            | cats vs rest | 2.913 | 3.284 | 3.283 | 2.633 | 3.891 | 2.712 | 4.597 | 4.758 |
|            | dogs vs rest | 2.863 | 2.964 | 3.559 | 2.752 | 3.556 | 2.721 | 4.073 | 4.017 |
|            | confidence | 5.834 | 4.935 | 5.681 | 5.122 | 5.945 | 6.346 | 7.138 | 6.778 |
| wide32     | cars vs rest | 1.491 | 2.075 | 1.774 | 1.673 | 2.116 | 1.572 | 3.128 | 2.857 |
|            | cats vs rest | 3.094 | 2.993 | 3.426 | 2.992 | 3.258 | 2.551 | 4.705 | 4.867 |
|            | dogs vs rest | 3.324 | 2.752 | 3.615 | 2.551 | 4.238 | 2.983 | 3.876 | 3.937 |
|            | confidence | 5.380 | 4.014 | 4.714 | 4.052 | 5.213 | 4.691 | 7.778 | 5.737 |

 avg rank: 3.3 3.0 4.3 2.3 5.2 2.9 7.7 7.2

### Table F16: Comparison of calibration evaluators in estimating the reliability diagram with $|\hat{c}_M - c^*|$ on CIFAR-5m. Table compares using the cross-validation with regularisation to no regularisation. Otherwise like Table F2.

| Model      | binning | $PL_{CE}^N - \text{notrick}$ | $PL_{CE}^E - \text{notrick}$ | $PL_{3CE}$ | $PL_{DE}^N - \text{notrick}$ | $PL_{DE}^E - \text{notrick}$ | $ES_{CV} - \text{notrick}$ | $ES_{CV}$ |
|------------|---------|-------------------------------|-------------------------------|-----------|-------------------------------|-------------------------------|-----------------------------|-----------|
| resnet110  | cars vs rest | 3.123 | 1.182 | 3.471 | 3.524 | 3.894 | 3.924 | 3.835 | 3.979 |
|            | cats vs rest | 7.575 | 7.441 | 7.814 | 7.723 | 10.157 | 10.173 | 10.045 | 10.044 |
|            | dogs vs rest | 6.562 | 6.371 | 7.035 | 7.041 | 8.875 | 8.975 | 9.299 | 9.079 |
|            | confidence | 9.952 | 9.791 | 10.711 | 11.094 | 11.535 | 11.767 | 14.146 | 13.866 |
| densenet40 | cars vs rest | 2.422 | 2.324 | 3.617 | 3.242 | 4.224 | 4.424 | 5.915 | 5.751 |
|            | cats vs rest | 5.682 | 5.724 | 7.164 | 7.164 | 7.76 | 7.76 | 9.252 | 9.127 |
|            | dogs vs rest | 5.212 | 5.021 | 6.747 | 6.797 | 6.911 | 6.946 | 8.222 | 8.022 |
|            | confidence | 10.669 | 10.725 | 11.541 | 11.053 | 11.686 | 11.781 | 13.093 | 12.557 |
| wide32     | cars vs rest | 2.591 | 2.624 | 3.886 | 3.898 | 3.684 | 3.691 | 3.584 | 3.596 |
|            | cats vs rest | 4.691 | 6.752 | 7.347 | 7.442 | 8.777 | 8.875 | 8.467 | 8.574 |
|            | dogs vs rest | 6.031 | 8.173 | 8.109 | 8.684 | 8.555 | 8.844 | 8.914 | 8.914 |
|            | confidence | 8.909 | 9.924 | 9.895 | 10.046 | 10.923 | 9.761 | 10.993 | 10.636 |

 avg rank: 1.6 1.4 3.7 4.3 5.8 5.8 6.5 6.6
Table F17: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_{M} - CE|$ on CIFAR-5m. Table compares using the cross-validation with regularisation to no regularisation. Otherwise like Table F4.

| Model     | binning | $PL_{\text{CE}}^{\text{M}}$ - notrick | $PL_{\text{CE}}^{\text{M}}$ | $PL_{\text{SE}}^{\text{M}} - notrick$ | $PL_{\text{SE}}^{\text{M}}$ | $PL_{\text{DE}} - notrick$ | $PL_{\text{DE}}$ | $ES_{\text{CV}} - notrick$ | $ES_{\text{CV}}$ |
|-----------|---------|---------------------------------------|-----------------------------|---------------------------------------|-----------------------------|-----------------------------|----------------|-----------------------------|----------------|
| resnet110 | cars vs rest | 1.92 | 2.08 | 1.35 | 1.36 | 1.78 | 1.84 | 2.81 | 2.84 |
|           | dogs vs rest | 3.14 | 3.35 | 2.72 | 2.75 | 3.34 | 3.26 | 4.02 | 4.06 |
| densenet40 | cats vs rest | 1.43 | 1.49 | 1.37 | 1.38 | 2.14 | 2.14 | 2.26 | 2.31 |
|           | dogs vs rest | 2.55 | 2.83 | 2.45 | 2.32 | 2.91 | 2.92 | 3.69 | 4.01 |
| wide32    | confidence | 5.62 | 5.97 | 5.86 | 5.21 | 5.53 | 5.31 | 6.41 | 6.73 |
| avg rank  |            | 4.7 | 5.2 | 2.5 | 2.7 | 4.2 | 4.2 | 6.3 | 7.2 |

Table F18: Comparison standard deviations of calibration evaluators in estimating the reliability diagram with $|\hat{c}_{M} - c^{*}|$ on CIFAR-5m. Otherwise like Table F2.

Table F19: Comparison of standard deviations of calibration evaluators in estimating the true calibration error with $|ECE_{M} - CE|$ on CIFAR-5m. Otherwise like Table F4.

In Table F23 Spearman correlation is used to see how well the measures are able to rank different models. All the measures are really good, the only exception is ‘stairs’, where Platt scaling and beta calibration are not as good.

F.3 Results of Real Experiments

Table F24 also shows the biases on the real data, to be compared with pseudo-real results. To achieve as valid results as possible, the pseudo-real data has the subset containing the architectures (Resnet110, WideNet32, Densenet40) and calibrated with the same methods (TempS, VecS, MSODIR, dirL2, dirODIR). The only difference is that real experiments are trained and evaluated on
Table F20: Comparison of calibration evaluators in estimating the reliability diagram with $|\hat{\mathcal{C}}_\mathcal{M} - C^*|$. Evaluated on synthetic data. The distance has been calculated on $10^6$ test data. The table displays thousandths.

| binning | $ES_{15}$ | $ES_{assoc}$ | $ES_{CV}$ | $PL_{20}^{CE}$ | $PL_{MSE}$ | $PL_{CE_{NN}}$ | $PL_{MSE_{NN}}$ | $PL_{DE}$ | Platt | beta | isotonic |
|---------|-----------|-------------|-----------|----------------|------------|----------------|----------------|----------|-------|-------|----------|
| square  | 24.76(1)  | 20.46(1)    | 17.33(6)  | 9.98(2)       | 10.98(3)   | 13.07(6)      | 12.78(5)      | 14.88(5) | 9.48(1)| 11.04(3)| 25.45(1) |
| sqrt    | 24.78(1)  | 20.43(1)    | 16.87(1)  | 13.29(6)      | 14.44(7)   | 13.45(6)      | 14.06(6)      | 13.04(6) | 11.82(1)| 11.18(3)| 25.45(1) |
| beta1   | 25.31(1)  | 20.98(1)    | 18.98(6)  | 14.76(4)      | 15.27(2)   | 16.87(6)      | 17.55(6)      | 13.69(6) | 11.32(1)| 12.49(2)| 25.45(1) |
| beta2   | 25.54(1)  | 21.52(4)    | 21.58(6)  | 14.51(4)      | 14.41(3)   | 15.26(5)      | 15.31(6)      | 18.49(6) | 12.87(1)| 14.33(3)| 25.45(1) |
| stairs  | 26.79(3)  | 23.24(4)    | 23.55(7)  | 18.72(3)      | 19.32(4)   | 17.89(5)      | 17.95(2)      | 20.09(6) | 50.44(1)| 36.14(1)| 25.45(8) |
| avg rank| 10.4       | 8.2         | 8.0       | 4.4           | 4.4        | 4.6            | 9.2           | 9.0       | 1.2   | 3.8    | 10.2     |

Table F21: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_\mathcal{M} - CE|$. Evaluated on synthetic data. The table displays thousandths.

| binning | $ES_{15}$ | $ES_{assoc}$ | $ES_{CV}$ | $PL_{20}^{CE}$ | $PL_{MSE}$ | $PL_{CE_{NN}}$ | $PL_{MSE_{NN}}$ | $PL_{DE}$ | Platt | beta | isotonic |
|---------|-----------|-------------|-----------|----------------|------------|----------------|----------------|----------|-------|-------|----------|
| square  | 7.41(3)   | 7.07(9)     | 6.59(6)   | 5.91(4)       | 6.31(6)    | 7.01(8)       | 6.98(7)       | 5.84(7)  | 5.79(1)| 5.81(3)| 8.66(1)  |
| sqrt    | 6.94(3)   | 6.58(6)     | 5.92(6)   | 6.37(4)       | 6.39(5)    | 7.12(10)      | 6.49(7)       | 6.21(7)  | 6.33(3)| 6.49(6)| 9.61(4)  |
| beta1   | 7.78(10)| 7.19(5)     | 7.11(6)   | 7.72(9)       | 6.83(5)    | 7.46(6)       | 6.96(7)       | 5.79(7)  | 6.76(2)| 6.95(4)| 10.38(1) |
| beta2   | 7.18(3)   | 8.04(6)     | 8.15(6)   | 8.34(10)      | 7.52(14)   | 7.75(5)       | 7.24(1)       | 6.88(7)  | 7.85(1)| 7.97(7)| 9.13(11) |
| stairs  | 7.12(1)   | 7.46(4)     | 7.29(6)   | 7.59(4)       | 7.58(6)    | 8.11(8)       | 7.32(4)       | 7.47(5)  | 29.27(1)| 24.98(10)| 10.39    |
| avg rank| 6.4       | 7.2         | 4.8       | 6.8           | 4.6        | 7.8           | 5.0           | 2.4      | 4.6   | 5.8   | 10.6     |

Table F22: Comparison of calibration evaluators in estimating the true calibration error with $|ECE_\mathcal{M} - CE|^2$. Evaluated on synthetic data. The table displays thousandths.

| binning | $ES_{15}$ | $ES_{assoc}$ | $ES_{CV}$ | $KCE$ | $PL_{20}^{CE}$ | $PL_{MSE}$ | $PL_{CE_{NN}}$ | $PL_{MSE_{NN}}$ | $PL_{DE}$ | Platt | beta | isotonic |
|---------|-----------|-------------|-----------|-------|----------------|------------|----------------|----------------|----------|-------|-------|----------|
| square  | 0.91(3)   | 0.97(10)   | 0.81(1)   | 1.62(2)| 0.69(1)       | 0.77(4)    | 0.81(2)       | 0.81(4)       | 0.83(4)  | 0.72  | 0.74  | 1.17(1)  |
| sqrt    | 0.81(4)   | 0.77(1)    | 0.76(2)   | 1.56(12)| 0.85(8)       | 0.74(1)    | 0.91(10)      | 0.79(2)       | 0.78(4)  | 0.89  | 0.85  | 1.39(11) |
| beta1   | 0.97(2)   | 0.92(4)    | 0.82(1)   | 4.01(12)| 0.97(10)      | 0.81(3)    | 0.94(3)       | 0.82(4)       | 0.74(1)  | 0.85  | 0.86  | 1.14(11) |
| beta2   | 1.03(5)   | 1.07(5)    | 0.96(2)   | 3.93(12)| 1.15(10)      | 1.06(7)    | 1.05(1)       | 1.05(2)       | 0.91(1)  | 1.06  | 1.06  | 1.25(11) |
| stairs  | 0.92(1)   | 0.91(1)    | 0.88(1)   | 4.11(12)| 1.02(7)       | 0.93(4)    | 1.06(4)       | 1.04(6)       | 0.95(2)  | 3.31  | 3.11  | 1.41(1)  |
| avg rank| 5.8       | 6.6        | 2.8       | 12.0    | 7.2           | 3.8        | 7.0            | 5.0            | 3.8      | 0.6   | 0.6   | 10.6     |

CIFAR-10, but the pseudo-real experiments are trained on CIFAR-5m dataset. To calculate average bias, one needs to subtract the average true calibration error from the average estimates - the same constant for each value in the row. For real data, we do not know this constant, but we have subtracted a value which makes the row average bias match with the corresponding row average bias of pseudo-real data. Thus, the true average biases are a constant shift away from these. However, as this does not affect the ranks, we can still compare whether the ranking of biases across different methods agrees between the synthetic and real data. There is a strong agreement, increasing confidence that the stronger methods on pseudo-real data in Tables F2 and F4 are also stronger on real data.

Figure F8 depicts how different evaluation methods order models by calibration. The results are shown for 10 different real model-dataset combinations. The test set size is 10k for each example. For each model-dataset combination there are 5 models after applying post-hoc calibration methods.
Table F23: Spearman correlations on synthetic data with uniform distribution.

| binning | $ES_{15}$ | $ES_{sweep}$ | $ES_{CV}$ | $PL^{CE}$ | $PL^{MSE}$ | $PL^{CE}_{NN}$ | $PL^{MSE}_{NN}$ | $PL_{DE}$ | Platt | beta | isotonic |
|---------|-----------|--------------|-----------|------------|------------|----------------|----------------|---------|-------|-------|---------|
| square  | 0.99654   | 0.989810     | 0.981111  | 0.99526    | 0.99652    | 0.991994       | 0.99548        | 0.99484  | 0.99541 | 0.99527 | 0.99651 |
| sqrt    | 0.987714  | 0.99371      | 0.984115  | 0.99312    | 0.99213    | 0.987894       | 0.98934        | 0.99165  | 0.99194 | 0.99130 | 0.98942 |
| beta1   | 0.99652   | 0.995545     | 0.99312   | 0.98424    | 0.97029    | 0.960131       | 0.956104       | 0.99455  | 0.99456 | 0.99741 | 0.99612 |
| beta2   | 0.99712   | 0.994211     | 0.99795   | 0.99844    | 0.99991    | 0.99873        | 0.99966        | 0.99746  | 0.99745 | 0.99589 | 0.994210 |
| stairs  | 0.99651   | 0.99562      | 0.98956   | 0.98888    | 0.98989    | 0.988794       | 0.99265        | 0.99454  | 0.95491 | 0.97775 | 0.99324 |

avg rank 0.9 0.6 1.0 1.6 5.9 4.9 2.2 2.9 0.0 1.3 0.4 1.8

Fig. F8: Ordering of models from the most to the least calibrated by estimated calibration error on real dataset models (shown as subfigures), according to different evaluation methods (shown as rows within the subfigures). Test set size is 10k for each dataset.

It can be seen from the figure that for all cases, the choice of the evaluation method has consequences on the ordering of models. For example, for resnet110SD_c100, beta, isotonic and Platt order vector scaling (VecS) as the most calibrated model, while other methods order temperature scaling (TempS) as the most calibrated model.

F.4 Running Time of the Experiments

The experiments were run on the pseudo-real data combining 13 calibration maps (6 was used for final results), 5 seeds, 3 models and 3 data sizes and 4 2-class experiments (3 1vsRest and 1 confidence). In total 2340 combinations for
Table F24: Bias calculated on the pseudo-real (CIFAR-5m) and real data. The asterisk (*) denotes that the center of real biases is unknown but they have been shifted to match the average bias of pseudo-real data covering the same 5 calibration functions and 3 models (DenseNet40, ResNet110, WideNet32). The table displays thousandths.

| binning | E_{15} | E_{sweep} | E_{CV} | PL^{ECE} | PL^{MK} | PL^{DE} | beta | isotonic | Platt |
|---------|--------|-----------|--------|----------|---------|---------|------|----------|-------|
| CIFAR-5m | 1000 | 2.280 | 1.160 | 2.641 | 4.341 | 1.251 | 4.372 | 2.611 | 0.111 | 4.762 | -0.400 |
| 3000 | -0.528 | -0.832 | 0.221 | -0.055 | 0.094 | 0.453 | 0.054 | 2.451 | -1.460 |
| Real Data* | 1000 | 2.485 | 0.062 | 1.302 | 6.472 | 1.997 | 3.853 | 2.169 | 8.111 | 2.454 |
| 3000 | 0.516 | -1.372 | 0.602 | 2.372 | 0.250 | 1.760 | 0.714 | 4.461 | 0.497 |
| 10000 | -0.257 | -1.424 | 0.142 | -0.034 | -0.226 | 0.292 | -0.111 | 1.651 | -0.584 |

all the ECE methods, isotonic, beta, platt, kernel methods and PL methods took around 6500 hours. Running the experiments on the synthetic data combining 5 calibration maps, 5 seeds, 21 derivates and 3 data sizes, for all the ECE methods, isotonic, beta, platt, kernel methods and PL methods took around 5000 hours. The experiments were run on the real data combining 11 model-dataset combinations, with three different data sizes with different number of subsets (total 10) and 5 calibration methods, in total 700 combinations, which took under 350 hours. The scripts were run in a high performance computing center using CPU processing power (Intel(R) Xeon(R) CPU E5-2660 v2 @ 2.20GHz) with up to 6GB of RAM.

Appendix G Limitations and Future Work

While piecewise linear methods in both the original probability space and in the logit-logit space have improved the state-of-the-art as calibrators and as evaluators of calibration, there is room for improvement: (1) we have not experimented on non-neural classification methods to identify whether PL or PL3 or some other method would work well there; (2) when estimating calibration error, PL and PL3 would benefit from debiasing methods to further improve performance; (3) the running time of PL and PL3 should be reduced, e.g. by only considering less bins (usually 5 or less bins were used) and using 3- or 5-fold CV instead of 10-fold CV; (4) new pseudo-real datasets should be created from generative models trained on other datasets than CIFAR-10, so that true calibration maps could be estimated and calibration methods compared; and (5) new calibration map families could be created based on results with new pseudo-real datasets.