ESD: EXPECTED SQUARED DIFFERENCE AS A TUNING-FREE TRAINABLE CALIBRATION MEASURE

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ABSTRACT

Recent studies have shown that modern neural networks tend to be poorly calibrated due to over-confident predictions. Traditionally, post-processing methods have been used to calibrate the model after training. On the other hand, various trainable calibration measures have been proposed recently to incorporate the calibration objective loss directly into the training process. However, these methods all incorporate internal hyperparameters introduced in the process of obtaining a differential calibration measure. Consequently, the performance of these calibration objectives relies on tuning these hyperparameters, incurring more computational cost as the size of neural networks and datasets become larger. As such, we present Expected Squared Difference (ESD), a tuning-free (i.e., hyperparameter-free) trainable calibration objective loss, where we view the calibration error from the perspective of the squared difference between two expectations. With extensive experiments on several architectures (MLPs, CNNs, Transformers) and datasets, we demonstrate that (1) incorporating ESD into the training improves model calibration in various batch size settings without the need for internal hyperparmeter tuning, (2) ESD yields the best calibrated results compared with previous approaches, (3) show that ESD drastically improve the computational cost required for calibration during training due to the absence of internal hyperparamater. Code will be publicly available.

1 INTRODUCTION

The calibration of a neural network measures the extent to which the predictions it makes align with the true probability distribution. Possessing this property becomes especially important in real-world applications, such as autonomous driving (Bojarski et al., 2016) and medical diagnosis (Kocbek et al., 2020), where uncertainty-based decisions of the neural network are crucial to guarantee the safety of the users. However, despite the success of modern neural networks in accurate classification, they are shown to be poorly calibrated due to the tendency of the network to make predictions with high confidence (i.e., over-confident predictions) (Guo et al., 2017).

Traditionally, post-processing methods have been used, such as temperature scaling and vector scaling (Guo et al., 2017), to calibrate the model using the validation set after the training by adjusting the logits prior to the final softmax layer. Recently, various trainable calibration objectives have been proposed, such as MMCE (Kumar et al., 2018) and SB-ECE (Karandikar et al., 2021), which are added to the loss function as a regularizer to jointly optimize accuracy and calibration during training. A key advantage of calibration during training is that it is possible to cascade post-processing calibration methods after training to achieve even better-calibrated models. Unfortunately, these existing approaches introduce additional hyperparameters in their proposed calibration objectives, and the performance of the calibration objectives is highly sensitive to these design choices. Therefore these hyperparameters need to be tuned carefully on a per model per dataset basis, which greatly reduces their viability for training on large models and datasets.

To this end, we propose Expected Squared Difference (ESD), a trainable calibration objective loss that is hyperparameter-free. ESD is inspired by the KS-Error (Gupta et al., 2020), and it views the calibration error from the perspective of the difference between two expectations. In detail, our contributions can be summarized as follows:

- We propose ESD as a trainable calibration objective loss that can be jointly optimized with the negative log-likelihood loss (NLL) during training. ESD is a binning-free calibration objective loss, and no additional hyperparamters are required. We also provide an unbiased estimator of the Expected Squared Difference, and show that it can be utilized in small batch train settings.
- With extensive experiments we demonstrate that across various architectures (MLPs, CNNs & Transformers) and datasets (in vision & NLP domains), ESD provides the best calibration results when compared to previous approaches. Calibrations of these models are further improved by post-processing methods.
- We show that due to the absence of an internal hyperparameter in ESD that needs to be tuned, it shows a drastic improvement compared to previous calibration objective losses with regards to the total computational cost for training. The discrepancy in computational cost between ESD and tuning-required calibration objective losses becomes larger as the model complexity and dataset size increases.

2 Related Work

Calibration of neural networks has gained much attention following the observation from Guo et al. (2017) that modern neural networks are poorly calibrated. One way to achieve better calibration is to design better neural network architectures tailored for uncertainty estimation, e.g., Bayesian Neural Networks (Blundell et al., 2015; Gal & Ghahramani, 2016) and Deep Ensembles (Lakshminarayanan et al., 2017). Besides model design, **post-processing** calibration strategies have been widely used to calibrate a trained machine learning model using a hold-out validation dataset. Examples include temperature scaling (Guo et al., 2017) which scales the logit output of a classifier with a temperature parameter; Platt scaling (Platt, 1999) which fits a logistic regression model on top of the logits; and Conformal prediction (Vovk et al., 2005; Lei et al., 2018) which uses validation set to estimate the quantiles of a given scoring function. Other post-processing techniques include histogram binning (Zadrozny & Elkan, 2001), isotonic regression (Zadrozny & Elkan, 2002), and Bayesian binning into quantiles (Pakdaman Naeini et al., 2015).

Our work focuses on **trainable calibration methods** which train neural networks using a hybrid objective, combining a primary training loss with an auxiliary calibration objective loss. In this regard, one popular objective is Maximum Mean Calibration Error (MMCE) (Kumar et al., 2018), which is a kernel embedding based measure of calibration that is differentiable and therefore suitable as a calibration objective loss. Moreover, Karandikar et al. (2021) proposes a trainable calibration objective loss, SB-ECE and S-AvUC which softens previously defined calibration measures.

3 Problem Setup

This section introduces the notion of calibration error in neural networks and the metric widely used to estimate it. We then introduce the framework and pre-existing problems of calibration during training. The notations defined in this section will be used throughout the paper.

3.1 Calibration Error and Metric

Let us first consider an arbitrary neural network as $f_\theta : \mathcal{D} \rightarrow [0,1]^k$ with network parameters θ, where $\mathcal{D}$ is the input domain and k is the number of classes in the multiclass classification task. Furthermore, we assume that the training data, $(\boldsymbol{x_i}, \boldsymbol{y_i})_{i=1}^n$ are sampled *i.i.d.* from the joint distribution $\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y})$ (here we use one-hot vector for $\boldsymbol{y}$). Here, $\boldsymbol{Y} = (Y_1, ..., Y_k)$, and $\boldsymbol{y} = (y_1, ..., y_k)$ are samples from this distribution. We can further define a multivariate random variable $\boldsymbol{Z} = f_\theta(\boldsymbol{X})$ as the distribution of the outputs of the neural network. Similarly, $\boldsymbol{Z} = (Z_1, ..., Z_k)$, and $\boldsymbol{z} = (z_1, ..., z_k)$ are samples from this distribution. We use $(z_{k,i}, y_{k,i})$ to denote the output confidence and the one-hot vector element associated with the k-th class of the i-th training sample. Using this formulation, a neural network is said to be perfectly calibrated for class k, if and only if

$$\mathbb{P}(Y_k = 1 | Z_k = z_k) = z_k. \tag{1}$$

Intuitively, Eq.(1) requires the model accuracy for class k to be z_k on average for the inputs where the neural network produces prediction of class k with confidence z_k. In many cases, the research of

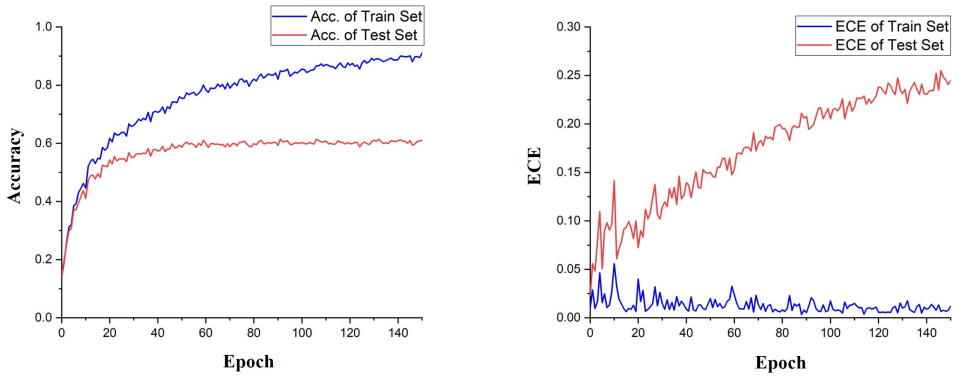

Figure 1: Accuracy curve (left) and its corresponding ECE curve (right) during training with negative log-likelihood (NLL) loss. It could be seen that since NLL implicitly trains for calibration error, the ECE of the train set approaches zero while the ECE of the test set increases during training.

calibration mainly focuses on the calibration of the max output class that the model predicts. Thus, calibration error is normally reported with respect to the predicted class (i.e., max output class) only. In the rest of the paper, for simplicity, k will denote the class with maximum output probability unless stated otherwise. Furthermore, we also write $I(\cdot)$ as the indicator function which returns one if the Boolean expression is true and zero otherwise.

With these notations, one common measurement of calibration error is the difference between confidence and accuracy which is mathematically represented as (Guo et al., 2017)

$$\mathbb{E}_{Z_k}\left[|\mathbb{P}(Y_k = 1|Z_k) - Z_k|\right]. \tag{2}$$

To estimate this, the Expected Calibration Error (ECE) (Naeini et al., 2015) uses B number of bins with disjoint intervals $B_j = (\frac{j}{B}, \frac{j+1}{B}]$, $j = 0, 1, ..., B-1$ to compute the calibration error as follows:

$$\text{ECE} = \frac{1}{|\mathcal{D}|}\sum_{j=0}^{B-1}\sum_{i=1}^{N}\left|I\left(\frac{j}{B} < z_{k,i} \leq \frac{j+1}{B}, y_{k,i} = 1\right) - z_{k,i})\right| \tag{3}$$

Kumar et al. (2018) and Karandikar et al. (2021) suggested that the disjoint bins in ECE can introduce discontinuities which are problematic when using it as a calibration objective loss in training. Therefore additional parameters were introduced to smooth it for the purpose of calibration during training.

3.2 Calibration During Training

Post-processing method and calibration during training are the two primary approaches for calibrating a neural network. Our focus in this paper is on the latter, where our goal is to train a calibrated yet accurate classifier directly. Note that calibration and predictive accuracy are independent properties of a classifier. In other words, being calibrated does not imply that the classifier has good accuracy and vice versa. Thus, training a classifier to have both high accuracy and good calibration requires jointly optimizing a calibration objective loss alongside the negative log-likelihood (NLL) with a scaling parameter λ for the secondary objective:

$$\min_{\theta} \text{NLL}(\mathcal{D}, \theta) + \lambda \cdot \text{CalibrationObjective}(\mathcal{D}, \theta). \tag{4}$$

3.2.1 Existing Trainable Calibration Objectives need Tuning

Various trainable calibration objectives have been proposed in the past. For example, Kumar et al. (2018) proposed Maximum Mean Calibration Error (MMCE), where it utilizes a Laplacian Kernel instead of the disjoint bins in ECE. Karandikar et al. (2021) proposed soft-binned ECE (SB-ECE)

and soft AvUC, which are softened versions of the ECE metric and the AvUC loss (Krishnan & Tickoo, 2020), respectively. All these approaches address the issue of discontinuity which makes the training objective differentiable. However they all introduce additional design choices - MMCE requires a careful selection of the kernel width ϕ, SB-ECE needs to choose the number of bins M and a softening parameter T, and S-AvUC requires a user-specified entropy threshold κ in addition to the softening parameter T. Searching for the optimal hyper-parameters can be computationally expensive especially as the size of models and dataset become larger.

3.2.2 Calibration During Training Suffers from Over-fitting Problem

NLL loss is known to implicitly train for calibration since it is a proper scoring rule, so models trained with NLL can overfit in terms of calibration error (Mukhoti et al., 2020; Karandikar et al., 2021). Figure 1 provides an example of an accuracy curve and its corresponding ECE curve for a model trained with NLL loss. We see that the model is overfitting in terms of both accuracy and ECE, which causes the gap between train and test ECE to become larger during training. As such, adding a calibration objective to the total loss will not be able to improve model calibration as it mainly helps improve calibration of the model with respect to the training data only.

Kumar et al. (2018) tackle this issue by introducing a weighted version of their calibration objective loss. They consider using larger weights to incorrect prediction samples after observing that the fraction of incorrect to the correct samples on the training data is smaller than that of the validation and test data. Instead of changing the calibration objective function itself, Karandikar et al. (2021) introduced a new training scheme called "interleaved training", where they split the training data further and dedicate a small portion of it to optimize the calibration objective loss. We will follow this strategy and introduce the technical details in the later sections.

4 ESD: Expected Squared Difference

We propose Expected Squared Difference (ESD) as a tuning-free (i.e., hyperparmeter-free) calibration objective. Our approach is inspired by the viewpoint of calibration error as a measure of distance between two distributions (Gupta et al., 2020)

In particular, we consider calibration error as difference between two expectations. We first start with the definition of perfect calibration in Eq.(1):

$$\begin{aligned} & \mathbb{P}(Y_k = 1 | Z_k = z_k) = z_k && \forall z_k \in [0,1] \\ \Leftrightarrow\ & \mathbb{P}(Y_k = 1, Z_k = z_k) = z_k \mathbb{P}(Z_k = z_k) && \forall z_k \in [0,1] \qquad \text{(Bayes rule).} \end{aligned} \tag{5}$$

Now considering the accumulation of the terms on both sides for arbitrary level $\alpha \in [0,1]$, perfect calibration for an arbitrary class k can now be written as:

$$\begin{aligned} & \int_0^\alpha \mathbb{P}(Y_k = 1, Z_k = z_k) dz_k = \int_0^\alpha z_k \mathbb{P}(Z_k = z_k) dz_k \\ \Leftrightarrow\ & \mathbb{E}_{Z_k, Y_k}[I(Z_k \leq \alpha, Y_k = 1)] = \mathbb{E}_{Z_k, Y_k}[Z_k I(Z_k \leq \alpha)], \quad \forall \alpha \in [0,1]. \end{aligned} \tag{6}$$

This allows us to write the difference between the two expectations as

$$\begin{aligned} d_k(\alpha) &= \left| \int_0^\alpha \mathbb{P}(Y_k = 1, Z_k = z_k) - z_k \mathbb{P}(Z_k = z_k) dz_k \right| \\ &= |\mathbb{E}_{Z_k, Y_k}[I(Z_k \leq \alpha)(I(Y_k = 1) - Z_k)]|, \end{aligned} \tag{7}$$

and $d_k(\alpha) = 0, \forall \alpha \in [0,1]$ if and only if the model is perfectly calibrated for class k. With this in mind, we propose ESD as the expected squared difference between the two expectations:

$$\mathbb{E}_{Z_k'}[\mathbb{E}^2_{Z_k, Y_k}[I(Z_k \leq Z_k')(I(Y_k = 1) - Z_k)]]. \tag{8}$$

This new metric is validated by the following theorem.

Theorem 1. $\mathbb{E}_{Z_k'}[\mathbb{E}^2_{Z_k, Y_k}[I(Z_k \leq Z_k')(I(Y_k = 1) - Z_k)]] = 0$ *iff. the model is perfectly calibrated.*

Proof. Since $d_k(Z'_k)^2 = \mathbb{E}^2_{Z_k,Y_k}[I(Z_k \leq Z'_k)(I(Y_k = 1) - Z_k)]$ is a non-negative random variable induced by Z'_k, $\mathbb{E}_{Z'_k}[d_k(Z'_k)^2] = 0$ iff. $\mathbb{P}(d_k(Z'_k) = 0) = 1$. Furthermore,

$$\mathbb{P}(d_k(Z'_k) = 0) = 1 \quad \Longleftrightarrow \quad d_k(\alpha) = 0 \quad \forall\alpha \text{ s.t. } \mathbb{P}(Z'_k = \alpha) \neq 0.$$

Thus

$$\mathbb{E}_{Z'_k}[d_k(Z'_k)^2] = 0 \text{ iff. } d_k(\alpha) = 0 \qquad \forall\alpha \text{ s.t. } \mathbb{P}(Z'_k = \alpha) \neq 0.$$

From lemma 1.1 below, we have $d_k(\alpha) = 0 \forall\alpha \in [0, 1]$ iff. $d_k(\alpha) = 0 \quad \forall\alpha$ s.t. $\mathbb{P}(Z'_k = \alpha) \neq 0$. Consequently, $\mathbb{E}_{Z'_k}[\mathbb{E}^2_{Z_k,Y_k}[I(Z_k \leq Z'_k)(I(Y_k = 1) - Z_k)]] = 0$ iff. the model is perfectly calibrated.

□

Lemma 1.1 *Let $\mathcal{I}$ be the support set of random variable Z_k, then $d_k(\alpha) = 0\ \forall\alpha \in \mathcal{I}$ iff. $d_k(\alpha) = 0$ $\forall\alpha \in [0, 1]$.*

Proof. The backward direction result is straight-forward, so we only prove for the forward direction: If $d_k(\alpha) = 0\ \forall\alpha \in \mathcal{I}$, then $d_k(\alpha) = 0\ \forall\alpha \in [0, 1]$. For arbitrary $\alpha' \in \mathcal{I}^c$, if $\alpha' < \min_{a\in\mathcal{I}} a$, then $\mathbb{P}(Z_k = z_k) = 0$ for all $z_k \leq \alpha'$ and thus $d_k(\alpha') = 0$. On the other hand, if $\alpha' > \max_{a\in\mathcal{I}} a$. Let $\alpha = \min_{a\in\mathcal{I}} |a - \alpha'|$, we have

$$\begin{aligned}
d_k(\alpha') &= |\int_0^{\alpha'} \mathbb{P}(Y_k = 1, Z_k = z_k) - z_k\mathbb{P}(Z_k = z_k)dz_k| \\
&= |\int_0^{\alpha'} \mathbb{P}(Y_k = 1|Z_k = z_k)\mathbb{P}(Z_k = z_k) - z_k\mathbb{P}(Z_k = z_k)dz_k| \\
&= |\int_0^{\alpha} \mathbb{P}(Y_k = 1|Z_k = z_k)\mathbb{P}(Z_k = z_k) - z_k\mathbb{P}(Z_k = z_k)dz_k \\
&\quad + \int_{\alpha}^{\alpha'} \mathbb{P}(Y_k = 1|Z_k = z_k)\mathbb{P}(Z_k = z_k) - z_k\mathbb{P}(Z_k = z_k)dz_k| \\
&= |\int_0^{\alpha} \mathbb{P}(Y_k = 1|Z_k = z_k)\mathbb{P}(Z_k = z_k) - z_k\mathbb{P}(Z_k = z_k)dz_k|(\mathbb{P}(Z_k = z_k) = 0 \text{ for } z_k > \alpha) \\
&= 0
\end{aligned}$$

Here, the fourth line of the above equation is 0 because of $\mathbb{P}(Z_k > \alpha) = 0$. □

4.1 An estimator for ESD

In this section, we use $(z_{k,i}, y_{k,i})$ to denote the output confidence and the one-hot vector element associated with the k-th class of the i-th training sample respectively. As the expectations in the true Expected Squared Difference (Eq.(8)) are intractable, we propose a Monte Carlo estimator for it which is unbiased. A common approach is to use a naive Monte Carlo sampling with respect to both the inner and outer expectations to give the following:

$$\begin{aligned}
&\mathbb{E}_{Z'_k}[\mathbb{E}^2_{Z_k,Y_k}[I(Z_k \leq Z'_k)(I(Y_k = 1) - Z_k)]] \approx \frac{1}{N}\sum_{i=1}^{N} \bar{g}_i{}^2 \\
&\text{where } \bar{g}_i = \frac{1}{N-1}\sum_{\substack{j=1\\ j\neq i}}^{N} g_{ij} \text{ and } g_{ij} = I(z_{k,j} \leq z_{k,i})[I(y_j = k) - z_{k,j}].
\end{aligned} \tag{9}$$

However, Eq. (9) results in a biased estimator that is an upper bound of the true Expected Squared Difference. To account for the bias, we propose the unbiased and consistent estimator (proof in Appendix A) of the true Expected Squared Difference,

$$ESD = \frac{1}{N}\sum_{i=1}^{N}\left[\bar{g}_i{}^2 - \frac{S^2_{g_i}}{N-1}\right] \quad \text{where } S^2_{g_i} = \frac{1}{N-2}\sum_{\substack{j=1\\ j\neq i}}^{N}(g_{ij} - \bar{g}_i)^2. \tag{10}$$

4.2 INTERLEAVED TRAINING

Negative log-likelihood (NLL) has be shown to greatly overfit to the ECE of the data it is trained on. Thus, training for calibration using the same data for the NLL has limited effect on reducing the calibration error of the model. Karandikar et al. (2021) proposed "Interleaved Training" where they split the train set into two subsets - one is used to optimize the NLL and the other is used to optimize the calibration objective. Following this framework, let $\mathcal{D}_{train}$ denote the entire train set. We separate the train set into two subsets - $\mathcal{D}'_{train}$ and $\mathcal{D}'_{cal}$. The joint training of ESD with NLL becomes,

$$\min_{\theta} \text{NLL}(\mathcal{D}'_{train}, \theta) + \lambda \cdot \text{ESD}(\mathcal{D}'_{cal}, \theta). \tag{11}$$

With this training scheme, NLL is optimized on $\mathcal{D}'_{train}$ and the ESD is optimized on $\mathcal{D}'_{cal}$. This way, Karandikar et al. (2021) showed that we can avoid minimizing ECE that is already overfit to the train set due to the NLL loss.

5 EXPERIMENTAL SETTING

5.1 DATASETS AND MODELS

We evaluate the proposed ESD metric as a trainable calibration objective on both image classification and natural language inference tasks.

Image Classification For image classification tasks we use the following datasets:

- MNIST (Deng, 2012): A large database of handwritten digit images (28x28). 54,000/6,000/10,000 images for train/validation/test split was used. We resized the images to (32x32) before inputting to the network.
- CIFAR10 & CIFAR100 (Krizhevsky et al., a;b): Color images (32x32) from 10 classes. 45,000/5,000/10,000 images for train/validation/test split was used. Used random cropping of 32 with padding of 4. Normalized each RGB channel with mean of 0.5 and standard deviation of 0.5.

Natural Language Inference (NLI) NLI is a task in Natural Language Processing where it involves classifying the inference relation (entailment, contradiction, or neutral) between two texts (MacCartney & Manning, 2008). For NLI tasks we use the following datasets:

- SNLI (Bowman et al., 2015): SNLI corpus is a collection of human-written English sentence pairs manually labeled for balanced classification with the labels entailment, contradiction, and neutral. The data consists of 550,152/10,000/10,000 sentence pairs for train/val/test set respectively. The max length of the input is set to 158.
- ANLI (Nie et al., 2019): ANLI dataset is a large-scale NLI benchmark dataset, collected via an iterative, adversarial human-and-model-in-the-loop procedure. The data consists of 162,865/3,200/3,200 sentence pairs for train/val/test set respectively. The max length of the input is set to 128.

For the MNIST dataset we used a MLP architecture, LeNet5 (Lecun et al., 1998). On CIFAR10 and CIFAR100 we used Convolutional Neural Networks (CNNs), ResNet50 and ResNet34 (He et al., 2015), respectively. Transformers, Bert-base (Devlin et al., 2018) and Roberta-base (Liu et al., 2019), has been used for SNLI and ANLI dataset respectively.

5.2 EXPERIMENTAL SETUP

We compare our Expected Squared Difference (ESD) to previously proposed trainable calibration objectives, MMCE and SB-ECE, on the datasets and models previously mentioned. For fair comparison, interleaved training has been used for all three calibration objectives. For MMCE, in which Kumar et al. (2018) proposed an unweighted and weighted version of the objective, we use the former to set the method to account for the overfitting problem mentioned in section 3.2.2 consistent to interleaved training. For the interleaved training settings, we held out 10% of the train set to the

	Loss Fn.	Dataset (Model)				
		MNIST (LeNet5)	CIFAR10 (Resnet50)	CIFAR100 (Resnet34)	SNLI (Bert-base)	ANLI (Roberta-base)
Acc.	NLL (baseline)	98.8±0.034	92.9±0.159	68.4±0.491	90.2±0.434	49.4±0.323
	+MMCE	98.4±0.320	91.5±0.340	66.5±0.644	89.4±0.491	49.0±0.471
	+SB-ECE	97.9±0.177	91.6±0.288	67.3±0.367	89.1±0.668	48.5±0.481
	+ESD (ours)	98.6±0.204	92.1±0.141	67.4±0.356	89.3±0.536	48.0±0.451
ECE	NLL (baseline)	0.91±0.080	5.49±0.105	23.8±0.403	4.20±0.420	35.9±0.505
	+MMCE	0.36±0.029	4.92±0.292	13.9±0.545	1.11±0.181	31.2±0.850
	+SB-ECE	0.41±0.067	4.86±0.319	14.7±1.370	1.82±0.301	33.9±1.378
	+ESD (ours)	**0.30**±0.035	**3.08**±0.692	**13.6**±0.950	**0.98**±0.165	**28.8**±0.543
ECE *after* TS	NLL (baseline)	0.31±0.044	1.89±0.105	5.74±0.306	1.04±0.112	4.16±0.445
	+MMCE	0.33±0.068	1.92±0.274	4.91±0.457	1.01±0.178	3.71±0.175
	+SB-ECE	0.45±0.103	1.63±0.300	4.94±0.240	0.99±0.180	3.98±0.733
	+ESD (ours)	**0.29**±0.030	**1.60**±0.089	**4.85**±0.390	**0.73**±0.192	**3.49**±0.373
Acc. *after* VS	NLL (baseline)	98.7±0.058	92.3±0.625	65.6±0.420	90.1±0.397	47.8±0.381
	+MMCE	98.4±0.250	91.3±0.429	66.3±0.773	89.5±0.588	47.7±0.429
	+SB-ECE	97.9±0.073	91.5±0.343	66.38±0.369	89.20±0.765	47.26±0.281
	+ESD (ours)	98.6±0.167	92.1±0.314	67.11±0.496	89.37±0.583	47.08±0.429
ECE *after* VS	NLL (baseline)	0.43±0.123	2.96±1.596	9.97±1.167	0.96±0.099	5.21±0.613
	+MMCE	0.32±0.055	2.52±0.586	4.59±1.575	1.08±0.170	4.79±0.693
	+SB-ECE	0.39±0.088	1.88±0.393	4.57±1.253	0.90±0.109	5.10±1.119
	+ESD (ours)	**0.28**±0.071	**1.61**±0.287	**4.28**±1.396	**0.61**±0.126	**4.42**±1.010

Table 1: Average accuracy and ECE (with std. across 5 trials) for baseline, MMCE, SB-ECE, and ESD after training and after post-processing with temperature scaling (TS) or vector scaling (VS).

calibration set. The regularizer hyperparameter λ for weighting the calibration measure with respect to NLL is chosen via fixed grid search [1]. For measuring calibration error, we use ECE with 20 equally sized bins. For the image classification tasks we use AdamW (Loshchilov & Hutter, 2017) optimizer with 10^{-3} learning rate and 10^{-2} weight decay for 250 epochs. For the NLI tasks, we use AdamW optimizer with 10^{-5} learning rate and 10^{-2} weight decay for 15 epochs. For both tasks, we use a batch size of 512.

The internal hyperparameters within MMCE (ϕ) and SB-ECE (M, T) were sequentially optimized [2] following the search for optimal λ. Following the original experimental setting of SB-ECE by Karandikar et al. (2021), we fix the hyperparameter M to 15. Similar to the model selection criterion utilized by Karandikar et al. (2021), we look at the accuracy and the ECE of all possible hyperparameter configurations in the grid. We choose the lowest ECE while giving up less than 1.5% accuracy relative to baseline accuracy on the validation set. All experiments were done using NVIDIA Quadro RTX 6000.

6 Experimental Result

In Table 1, we report the accuracy and ECE before and after post-processing (i.e., temperature scaling and vector scaling) of various datasets and models. Compared to the baseline or other trainable calibration objective loss (MMCE and SB-ECE), jointly training with ESD as the secondary loss consistently results in a better-calibrated network for all the datasets and models with around 1% degradation of accuracy. Moreover, we observe that applying post-processing (i.e., temperature scaling (TS) and vector scaling (VS)) after training with a calibration objective loss generally results in better-calibrated models over baseline post-processing, in which case ESD still outperforms other methods. Comparing the calibration outcomes in temperature scaling with vector scaling for models trained with ESD, vector scaling worked better as a post-processing method with minimal impact on the accuracy for all datasets except for ANLI, in which case the accuracy after vector scaling decreased more than 2%.

[1] For λ, we search for [0.2, 0.4, 0.6, 0.8, 1.0, 2.0, 3.0, ... 10.0].

[2] For ϕ, we search [0.2, 0.4, 0.6, 0.8]. For T, we search [0.0001, 0.001, 0.01, 0.1].

We show in Figure 2 that across different models and datasets the calibration performance of MMCE and SB-ECE is sensitive to the internal hyperparmater. This shows the importance of hyperparameter tuning in these methods. On the other hand, ESD does not only outperforms MMCE and SB-ECE in terms of ECE but does not have an internal hyperparameter to tune for.

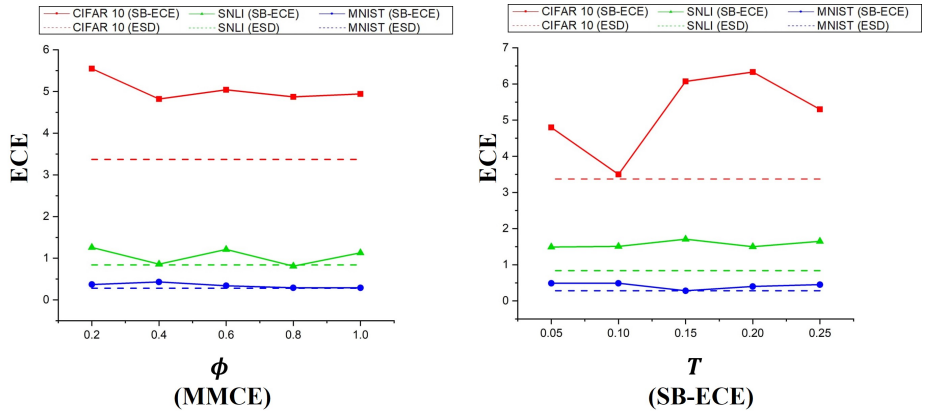

Figure 2: ECE performance curve of MMCE (left) and SB-ECE (right) with respect to their varying internal hyperparameters on MNIST, CIFAR10, SNLI datasets. Since the optimal hyperparameter changes for different models and datasets, they require a tuning process. On the other hand, our proposed ESD not only outperforms MMCE and SB-ECE but does not have an internal hyperparameter to tune for.

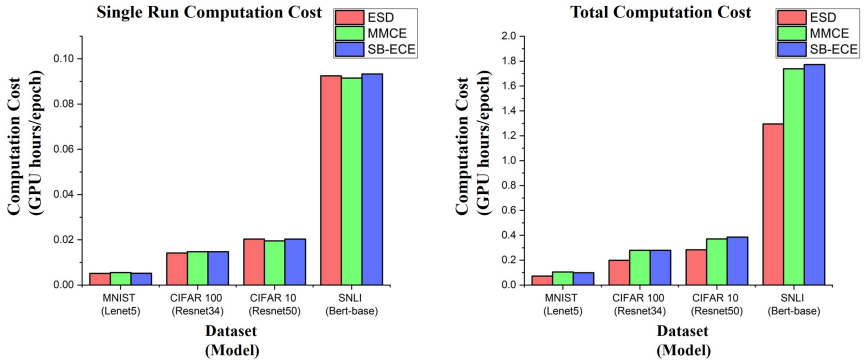

Figure 3: Computational cost of single-run training (left) and total cost considering hyperparameter tuning (right). The x-axis in both cases are in the order of increasing model complexity.

7 Ablation Study

7.1 Computational Cost of Hyperparameter Seach

We investigate the computational cost required to train a model with ESD compared to MMCE and SB-ECE. As depicted in Figure 3, the computational cost required to train a model for a single run remains nearly identical across different models and datasets. However, considering the need for tuning additional hyperparameters within MMCE and SB-ECE, the discrepancy in total computational cost between ESD and tuning-required calibration objective losses becomes more prominent as the model complexity and dataset size increases.

7.2 Batch Size Experiments

Table 2 shows that ESD is robust to varying batch sizes which could be the byproduct of the fact that it is an unbiased and consistent estimator. This is because, regardless of batch size, being unbiased

guarantees that the average of the gradient vectors of ESD equals the gradient of the true estimate (See Appendix B).

Dataset (Model)	Loss Fn.	Acc.	ECE	ECE *after* TS	Acc. *after* VS	ECE *after* VS
CIFAR10 (Resnet50)	NLL (b512)	92.9±0.159	5.49±0.105	1.89±0.105	92.3±0.625	2.96±1.596
	+ESD (b512)	92.1±0.141	3.08±0.692	1.60±0.089	92.1±0.314	1.61±0.287
	+ESD (b256)	91.5±0.137	3.15±0.587	1.61±0.073	91.9±0.573	1.60±0.082
	+ESD (b128)	91.5±0.519	2.93±0.539	1.70±0.600	91.7±0.246	2.20±0.584
	+ESD (b64)	91.3±0.753	3.91±0.847	1.87±0.132	91.5±0.257	2.65±1.48
SNLI (Bert-base)	NLL (b512)	90.2±0.434	4.20±0.420	1.04±0.112	90.1±0.397	0.96±0.099
	+ESD (b512)	89.3±0.536	0.98±0.165	0.73±0.192	89.4±0.583	0.61±0.126
	+ESD (b256)	89.9±0.314	1.11±0.236	0.76±0.241	88.9±0.146	0.62±0.147
	+ESD (b128)	89.8±0.435	0.99±0.244	0.68±0.190	89.6±0.490	0.58±0.187
	+ESD (b64)	89.1±0.660	1.06±0.285	0.83±0.260	88.8±0.672	0.81±0.153

Table 2: Average accuracy and ECE (with std. across 5 trials) for ESD after training with batch sizes 64, 128, 256, and 512.

7.3 Are Indicator Functions Trainable?

Recent papers, Kumar et al. (2018) and Karandikar et al. (2021), have suggested that ECE is not suitable for training as a result of its high discontinuity due to binning, which can be seen as a form of an indicator function. However, the results from our method suggest that our measure was still able to train well despite the existence of indicator functions. In addition, previous measures also contain indicator functions in the form of *argmax* function that introduces discontinuities but remains to be trainable. As such, this brings to raise the question of whether calibration measures with indicator functions can be used for training. To investigate this, we ran ECE as an auxiliary calibration objective loss on different batch sizes and observed its performance.

We found that ECE, contrary to previous belief, is trainable under large batch sizes and not trainable under small batch sizes while ours maintains good performance regardless of batch size. The poor performance of ECE under small batch size setting could potentially be attributed to the high bias present in such cases. From this, it seems to suggest that indicator functions do not seem to inhibit the training of calibration.

Loss Fn.	Acc.	ECE
NLL (b512)	68.6±0.034	22.4±0.105
+ECE (b512)	68.2±0.025	14.6±0.252
+ECE (b256)	67.9±0.057	18.1±0.552
+ECE (b128)	68.1±0.084	21.0±0.552

Table 3: Average accuracy and ECE (with std. across 5 trials) for ECE after training with batch sizes 128, 256, and 512.

8 Conclusions

Motivated by the need for a tuning-free trainable calibration objective, we proposed Expected Squared Difference (ESD), which does not contain any internal hyperparameters. With extensive comparison with existing methods for calibration during training across various architectures (MLPs, CNNs Transformers) and datasets (in vision & NLP domains), we demonstrate that training with ESD provides the best-calibrated models compared to other methods. Furthermore, the calibration of these models are further improved after post-processing. In addition, we demonstrate that ESD can be utilized in small batch settings while maintaining performance. More importantly, in contrast to previously proposed trainable calibration objectives, ESD does not contain any internal hyperparameters, which significantly reduces the total computational cost for training. This reduction in cost is more prominent as the complexity of the model and dataset increases, making ESD a more viable calibration objective option in modern deep learning settings.

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A PROOF THAT ESD IS AN UNBIASED AND CONSISTENT ESTIMATOR

In Theorem 2, we prove that ESD is an unbiased estimator, that is taking the expectation of ESD is equal to the true Expected Squared Difference.

Theorem 2 *ESD is an unbiased estimator, i.e.* $\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[ESD] = \mathbb{E}_{Z'_k}[d_k^2(Z'_k)]]$ *where* $d_k(Z'_k) = |\mathbb{E}_{Z_k,Y_k}[I(Z_k \leq Z'_k)(I(Y_k = 1) - Z_k)]|$

Proof. Let $\boldsymbol{Z_k}$=($Z_{k,1}$,...,$Z_{k,n}$), $\boldsymbol{Y_k}$ = ($Y_{k,1}$,...,$Y_{k,n}$) and $G_i = \bar{g_i}^2 - \frac{S^2_{g_i}}{N-1}$. We have that

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[ESD] &= \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[G_i] \quad \text{(by linearity of expectation)} \\
&= \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}_{Z_{k,i},Y_{k,i}}[\mu_i^2] \quad \text{(by lemma 2.1)} \\
&= \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}_{Z'_k}[d_k^2(Z'_k)]] \quad \text{(since } \mathbb{E}_{Z_{k,i},Y_{k,i}}[\mu_i^2] = \mathbb{E}_{Z'_k}[d_k^2(Z'_k))] \\
&= \mathbb{E}_{Z'_k}[d_k^2(Z'_k)]]]
\end{aligned}$$

□

Lemma 2.1 $\mathbb{E}_{\boldsymbol{Z_{k,-i}},\boldsymbol{Y_{k,-i}}}[G_i] = \mu_i^2$ *where* $\mu_i = \mathbb{E}_{Z_k,Y_k}[I(Z_k \leq Z_{k,i})(I(Y_k = 1) - z_k)]$

Proof. Since samples are i.i.d., for a fixed i, it holds that:

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{Z_{k,-i}},\boldsymbol{Y_{k,-i}}}[\bar{g}_i] &= \mu_i, \\
\mathbb{E}_{\boldsymbol{Z_{k,-i}},\boldsymbol{Y_{k,-i}}}[\frac{S^2_{g_i}}{N-1}] &= \frac{\sigma_i^2}{N-1} \quad \text{(where Var}[g_i] = \sigma_i^2) \\
\text{Var}[\bar{g}_i] &= \mathbb{E}_{\boldsymbol{Z_{k,-i}},\boldsymbol{Y_{k,-i}}}[\bar{g_i}^2] - \mu_i^2,
\end{aligned}$$

Shifting variables around, we get

$$\begin{aligned}
\mu_i^2 &= \mathbb{E}_{\boldsymbol{Z_{k,-i}},\boldsymbol{Y_{k,-i}}}[\bar{g_i}^2] - \text{Var}[\bar{g}_i] \\
&= \mathbb{E}_{\boldsymbol{Z_{k,-i}},\boldsymbol{Y_{k,-i}}}\left[\bar{g_i}^2 - \frac{S^2_{g_i}}{N-1}\right] \quad \text{(since Var}[\bar{g}_i] = \frac{\sigma_i^2}{N-1}) \\
&= \mathbb{E}_{\boldsymbol{Z_{k,-i}},\boldsymbol{Y_{k,-i}}}[G_i]
\end{aligned}$$

□

In Theorem 3, we prove that ESD is a consistent estimator, which means that ESD converges in probability to the true Expected Squared Difference.

Theorem 3 *ESD is a consistent estimator, i.e. ESD* $\xrightarrow{\mathbb{P}} \mathbb{E}_{Z'_k}[d_k^2(Z'_k)]$

Proof. Since ESD is an unbiased estimator, it is sufficient to prove $\lim_{n\to\infty}$ Var$[ESD] = 0$
For simplicity, we use where $\sum_{i,j=1}^{N} = \sum_{i=1}^{N}\sum_{j=1}^{N}$ and $\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[G_i] = \mathbb{E}_{Z'_k}[d_k^2(Z'_k)]\ \forall i$,

$$\text{Var}[ESD] = \frac{1}{N^2}\sum_{i=1}^{N}\text{Var}[G_i] + \frac{1}{N^2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\text{Cov}[G_i, G_j] \quad \text{where } \sum_{i,j=1}^{N} g_{i,j} = \sum_{i=1}^{N}\sum_{j=1}^{N} g_{i,j}$$

Since $\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[G_i] = \mathbb{E}_{Z'_k}[d_k^2(Z'_k)]\ \forall i$,

$$\begin{aligned}
&= \frac{1}{N^2}\sum_{i=1}^{N}\text{Var}[G_i] + \frac{1}{N^2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[G_iG_j] - \mathbb{E}^2_{Z'_k}[d_k^2(Z'_k)] \\
&\leq \frac{1}{N^2}\sum_{i=1}^{N} 2 + \frac{1}{N^2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}(\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\bar{g_i}^2\bar{g_j}^2] - \mathbb{E}^2_{Z'_k}[d_k^2(Z'_k)]) \quad \text{(by lemma 3.1 and 3.2)} \\
&+ \frac{1}{N^2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{4}{N-2} + \frac{4}{(N-2)^2} \\
&= \frac{2}{N} + \frac{4N(N-1)}{N^2(N-2)^2} + \frac{4N(N-1)}{N^2(N-2)} \quad \text{(by lemma 3.3)} \\
&+ \frac{N(N-1)}{N^2}(\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\bar{g_1}^2\bar{g_2}^2] - \mathbb{E}^2_{Z'_k}[d_k^2(Z'_k)])
\end{aligned}$$

Thus, by using lemma 3.4 and the non-negativeness of variance,

$$0 \leq \lim_{n\to\infty}\text{Var}[ESD] \leq \lim_{n\to\infty}\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\bar{g_1}^2\bar{g_2}^2] - \mathbb{E}^2_{Z'_k}[d_k^2(Z'_k)] = 0.$$

Consequently, $\lim_{n\to\infty}\text{Var}[ESD] = 0$

□

Lemma 3.1 *Var*$[G_i] \leq 2 < \infty$

Proof.

$$\begin{aligned}
\text{Var}[G_i] &= \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[G_i^2] - \mathbb{E}^2_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[G_i] \\
&\leq \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[G_i^2] \\
&= \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}\left[\bar{g_i}^2 - 2\frac{S^2_{g_i}}{N-1} + \left(\frac{S^2_{g_i}}{N-1}\right)^2\right] \\
&\leq \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}\left[\bar{g_i}^2 + \left(\frac{S^2_{g_i}}{N-1}\right)^2\right]
\end{aligned}$$

By lemma 3.2, $\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[g_i^2] \leq 1$ and $\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}\left[\left(\frac{S^2_{g_i}}{N-1}\right)^2\right] \leq \left(\frac{2}{N-2}\right)^2 \leq 1$. Thus, $\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}\left[\bar{g_i}^2 + \left(\frac{S^2_{g_i}}{N-1}\right)^2\right] \leq 2$.

□

Lemma 3.2 $|\frac{S^2_{g_i}}{N-1}| \leq \frac{2}{N-2}$ *and* $|\bar{g_i}| \leq 1$

Proof. By the triangle inequality, $|\bar{g}_i| = |\frac{1}{N-1}\sum_{\substack{m=1\\m\neq i}}^{N} g_{im}| \leq \frac{1}{N-1}\sum_{\substack{m=1\\m\neq i}}^{N} |g_{im}|$. It is upper bounded by one because $\forall m\ |g_{im}| \leq 1$. Furthermore, we have

$$\begin{aligned}
\left|\frac{S_{g_i}^2}{N-1}\right| &= \frac{1}{(N-1)^2}\sum_{\substack{m=1\\m\neq i}}^{N} g_{im}^2 + \frac{1}{(N-1)^2(N-2)}(\sum_{\substack{m=1\\m\neq i}}^{N} g_{im})^2 \\
&\leq \frac{1}{(N-1)^2}\sum_{\substack{m=1\\m\neq i}}^{N} |g_{im}|^2 + \frac{1}{(N-1)^2(N-2)}(\sum_{\substack{m=1\\m\neq i}}^{N} |g_{im}|)^2 \\
&\leq \frac{1}{(N-1)^2}\sum_{\substack{m=1\\m\neq i}}^{N} 1 + \frac{1}{(N-1)^2(N-2)}(\sum_{\substack{m=1\\m\neq i}}^{N} 1)^2
\end{aligned}$$

The last inequality is by $\forall m$, $|g_{im}| \leq 1$, and the direct calculation implies that

$$\left|\frac{S_{g_i}^2}{N-1}\right| \leq \frac{1}{N-1} + \frac{1}{N-2} \leq \frac{2}{N-2}.$$

□

Lemma 3.3 $\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\bar{g_i}^2\bar{g_j}^2] = \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\bar{g_1}^2\bar{g_2}^2]\ \forall i,j$ *where* $i \neq j$

Proof.

$$\begin{aligned}
\sum_{\substack{m,n=1\\\{m,n\}\neq\{i,j\}}}^{N} g_{im}g_{jn} &= \sum_{\substack{m,n=1\\\{m,n\}\neq\{i,j\},\, m\neq n}}^{N} g_{im}g_{jn} + \sum_{\substack{m,n=1\\n\neq\{i,j\}}}^{N} g_{ij}g_{jn} + \sum_{\substack{m,n=1\\m\neq\{i,j\}}}^{N} g_{im}g_{ji} \\
&\quad + \sum_{\substack{m,n=1\\m\neq\{i,j\}}}^{N} g_{im}g_{jm} + g_{ij}g_{ji} \qquad \text{(since these terms are disjoint terms)} \\
&\overset{d}{=} \sum_{\substack{m',n'=1\\\{m',n'\}\neq\{1,2\},\, m'\neq n'}}^{N} g_{1m'}g_{2n'} + \sum_{\substack{m',n'=1\\n'\neq\{1,2\}}}^{N} g_{12}g_{2n'} + \sum_{\substack{m',n'=1\\m'\neq\{1,2\}}}^{N} g_{1m'}g_{21} \\
&\quad + \sum_{\substack{m',n'=1\\m'\neq\{1,2\}}}^{N} g_{1m'}g_{2m'} + g_{12}g_{21} \\
&= \sum_{\substack{m',n'=1\\m'\neq 1, n'\neq 2}}^{N} g_{1m'}g_{2n'}
\end{aligned}$$

Proof of claim above:
As the summation can be divided into five distinct cases,

Let i and j be arbitrary such that $i \neq j$,

Case 1: $\{m, n\} \neq \{i, j\}$ and $m \neq n$

$$\begin{aligned} g_{im}g_{jn} &= I(Z_{k,m} \leq Z_{k,i})[I(Y_{k,m} = 1) - Z_{k,m}]I(Z_{k,n} \leq Z_{k,j})[I(Y_{k,n} = 1) - Z_{k,n}] \\ &= h_1(Z_{k,i}, Z_{k,m}, Z_{k,j}, Z_{k,n}, Y_{k,m}, Y_{k,n}) \\ &\overset{d}{=} h_1(Z_{k,1}, Z_{k,m'}, Z_{k,2}, Z_{k,n'}, Y_{k,m'}, Y_{k,n'}) \qquad \text{where } \{m', n'\} \neq \{1, 2\} \text{ and } m' \neq n' \end{aligned}$$

Case 2: $m = j$ and $n \neq \{i, j\}$

$$\begin{aligned} g_{ij}g_{jn} &= I(Z_{k,j} \leq Z_{k,i})[I(Y_{k,j} = 1) - Z_{k,j}]I(Z_{k,n} \leq Z_{k,j})[I(Y_{k,n} = 1) - Z_{k,n}] \\ &= h_2(Z_{k,i}, Z_{k,j}, Z_{k,n}, Y_{k,j}, Y_{k,n}) \\ &\overset{d}{=} h_2(Z_{k,1}, Z_{k,2}, Z_{k,n'}, Y_{k,2}, Y_{k,n'}) \qquad \text{where } m' = 2 \text{ and } n' \neq \{1, 2\} \end{aligned}$$

Case 3: $n = i$ and $m \neq \{i, j\}$

$$\begin{aligned} g_{im}g_{ji} &= I(z_{k,m} \leq Z_{k,i})[I(Y_{k,m} = 1) - Z_{k,m}]I(Z_{k,i} \leq Z_{k,j})[I(Y_{k,i} = 1) - Z_{k,i}] \\ &= h_3(Z_{k,i}, Z_{k,m}, Z_{k,j}, Y_{k,m}, Y_{k,i}) \\ &\overset{d}{=} h_3(Z_{k,1}, Z_{k,m'}, Z_{k,2}, Y_{k,m'}, Y_{k,1}) \qquad \text{where } n' = 1 \text{ and } m' \neq \{1, 2\} \end{aligned}$$

Case 4: $m = n \neq \{i, j\}$

$$\begin{aligned} g_{im}g_{jm} &= I(Z_{k,m} \leq Z_{k,i})[I(Y_{k,m} = 1) - Z_{k,m}]I(Z_{k,m} \leq Z_{k,j})[I(Y_{k,m} = 1) - Z_{k,m}] \\ &= h_4(Z_{k,i}, Z_{k,m}, Z_{k,j}, Y_{k,m}) \\ &\overset{d}{=} h_4(Z_{k,1}, Z_{k,m'}, Z_{k,2}, Y_{k,m'}) \qquad \text{where } m' = n' \neq \{1, 2\} \end{aligned}$$

Case 5: $m = j$ and $n = i$

$$\begin{aligned} g_{ij}g_{ji} &= I(Z_{k,j} \leq Z_{k,i})[I(Y_{k,j} = 1) - Z_{k,j}]I(Z_{k,i} \leq Z_{k,j})[I(Y_{k,i} = 1) - Z_{k,i} \\ &= h_5(Z_{k,i}, Z_{k,j}, Y_{k,i}, Y_{k,j}) \\ &\overset{d}{=} h_5(Z_{k,1}, Z_{k2}, Y_{k,1}, Y_{k,2}) \qquad \text{where } m' = 2 \text{ and } n' = 1 \end{aligned}$$

This follows from the fact that $Z_{k,i}$'s abd $Y_{k,i}$'s are i.i.d. random variables.
Therefore,

$$(\sum_{\substack{m,n=1 \\ m \neq i, n \neq j}}^{N} g_{im}g_{jn})^2 \overset{d}{=} (\sum_{\substack{m',n'=1 \\ m' \neq 1, n' \neq 2}}^{N} g_{1m'}g_{2n'})^2$$

$$\bar{g_i}^2 \bar{g_j}^2 \overset{d}{=} \bar{g_1}^2 \bar{g_2}^2$$

$$\mathbb{E}_{\boldsymbol{Z_k}, \boldsymbol{Y_k}}[\bar{g_i}^2 \bar{g_j}^2] = \mathbb{E}_{\boldsymbol{Z_k}, \boldsymbol{Y_k}}[\bar{g_1}^2 \bar{g_2}^2]$$

□

Lemma 3.5 $\lim_{N \to \infty} \mathbb{E}_{\boldsymbol{Z_k}, \boldsymbol{Y_k}}[\bar{g_1}^2 \bar{g_2}^2] = \mathbb{E}^2_{Z'_k}[d_k^2(Z'_k)]$

Proof. For arbitrary i, $\bar{g_i} \overset{\mathbb{P}}{\to} \mu_i$ by the strong law of large number. Thus, $\bar{g_1} \overset{\mathbb{P}}{\to} \mu_1$ and $\bar{g_2} \overset{\mathbb{P}}{\to} \mu_2$. Therefore, since marginal convergence in probability implies joint convergence in probability (Vaart, 1998),

$$(\bar{g_1}, \bar{g_2}) \quad \overset{\mathbb{P}}{\to} \quad (\mu_1, \mu_2)$$

By continuous mapping theorem, since $f(x, y) = x^2y^2$ is a continuous function,

$$\bar{g_1}^2 \bar{g_2}^2 \quad \overset{\mathbb{P}}{\to} \quad \mu_1^2 \mu_2^2$$

Additionally, since $|\bar{g_1}^2 \bar{g_2}^2| \leq 1 \; \forall N$, it is uniformly bounded and thus uniformly integrable. Combining this with the fact that it converges in probability,

$$\lim_{N \to \infty} \mathbb{E}_{\boldsymbol{Z_k}, \boldsymbol{Y_k}}[\bar{g_1}^2 \bar{g_2}^2] = \mathbb{E}_{\boldsymbol{Z_k}, \boldsymbol{Y_k}}[\mu_1^2 \mu_2^2]$$

Thus,

$$\lim_{N\to\infty} \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\bar{g_1}^2\bar{g_2}^2] = \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\mu_1^2\mu_2^2] = \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\mu_1^2]E_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[\mu_2^2] = \mathbb{E}^2_{Z'_k}[d_k^2(Z'_k)]$$

□

B UNBIASED ESTIMATORS AND ITS GRADIENT

Since ESD is an unbiased estimator,

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[ESD] &= \mathbb{E}_{Z'_k}[d_k^2(Z'_k)] \\
\nabla_\theta \mathbb{E}_{Z'_k}[d_k^2(Z'_k)] &= \nabla_\theta \mathbb{E}_{\boldsymbol{Z_k},\boldsymbol{Y_k}}[ESD] \\
&= \nabla_\theta \mathbb{E}_{\boldsymbol{X},\boldsymbol{Y}}[ESD] \qquad \text{(by law of unconscious statistician)} \\
&= \mathbb{E}_{\boldsymbol{X},\boldsymbol{Y}}[\nabla_\theta ESD] \qquad \text{(since } (\boldsymbol{X},\boldsymbol{Y}) \text{ are independent of } \theta)
\end{aligned}$$

Thus, the gradient of the unbiased estimator is on average the gradient of the desired metric.