

Comparing Correction Methods for Misclassification Bias

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Abstract. When applying supervised machine learning algorithms to classification, the classical goal is to reconstruct the true labels as accurately as possible. However, if the predictions of an accurate algorithm are aggregated, for example by counting the predictions of a single class label, the result is often still statistically biased. Implementing machine learning algorithms in the context of official statistics is therefore impeded. The statistical bias that occurs when aggregating the predictions of a machine learning algorithm is referred to as misclassification bias. In this paper, we focus on reducing the misclassification bias of binary classification algorithms by employing five existing estimation techniques, or estimators. As reducing bias might increase variance, the estimators are evaluated by their mean squared error (MSE). For three of the estimators, we are the first to derive an expression for the MSE in finite samples, complementing the existing asymptotic results in the literature. The expressions are then used to compute decision boundaries numerically, indicating under which conditions each of the estimators is optimal, i.e., has the lowest MSE. Our main conclusion is that the calibration estimator performs best in most applications. Moreover, the calibration estimator is unbiased and it significantly reduces the MSE compared to that of aggregated predictions, supporting the use of machine learning in the context of official statistics.[‡]

Keywords: Misclassification Bias · Supervised Machine Learning · Classification · Official Statistics

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[‡]The views expressed in this paper are those of the authors and do not necessarily reflect the policy of Statistics Netherlands.

1 Introduction

Currently, many researchers in the field of official statistics are examining the potential of machine learning algorithms. A typical example is estimating the proportion of houses in the Netherlands having solar panels, by employing a machine learning algorithm trained to classify satellite images [3]. However, as long as the algorithm’s predictions are not error-free, the estimate of the relative occurrence of a class, or *base rate*, can be distorted [14,15]. This fact is also intuitively clear: if the number of false positives does not equal the number of false negatives, then the estimate of the base rate is biased, even if the false positive rate and false negative rate are both small. In this paper, the statistical bias that occurs when aggregating the predictions of a machine learning algorithm is referred to as misclassification bias.

Misclassification bias when aggregating predictions occurs in a broad range of applications, including official statistics [11], land cover mapping [10], political science [7,17], and epidemiology [6]. The objective in each of these applications is to minimize a loss function at the level of aggregated predictions, in contrast to minimizing a loss function at the level of individual predictions. Within the field of machine learning, learning with that objective is referred to as quantification learning, see [4] for a recent overview. In quantification learning, the idea is not to train a classifier at all, but to directly estimate the base rate from the feature distribution. A drawback of that approach is that relatively large training and test datasets are needed to optimize hyperparameters and to obtain accurate estimates of the accuracy of the prediction, respectively. In the applications referred to before, labelled data are often expensive to obtain and therefore scarce. Hence, in this paper, we use the aggregated predictions of classification algorithms and investigate how to reduce the misclassification bias most effectively.

In the scientific literature on measurement error, several methods have been proposed to reduce misclassification bias when aggregating categorical data that is prone to measurement error, see [9] for a technical discussion and [1] for a more recent overview. Based on that literature, we propose a total of five estimators for the base rate that can be derived from the *confusion matrix* of a classification algorithm, see Table 1. As reducing bias might increase variance, the estimators are evaluated by their mean squared error (MSE). To the best of our knowledge, for three of the five estimators, only asymptotic expressions for the MSE are ever presented in the literature. In this paper, we derive the expressions for the MSE for finite datasets. As a first step, we restrict ourselves to binary classification problems. Nonetheless, we believe that the same proof strategies may be used for multi-class classification problems. The expressions for the MSE enable a theoretical comparison of the five estimators for finite datasets. It allows us, for the first time, to make solid recommendations on how to employ machine learning algorithms in the context of official statistics.

The remainder of the paper is organized as follows. First, in Section 2, the five estimators are formally introduced and the mathematical expressions for their MSEs are presented. The derivations are included in the appendix. Then,

Table 1: Crosstables for test set (left) and unlabeled data (right)

(a)		Estimated class			(b)		Estimated class		
		0	1	Tot			0	1	Tot
True class	0	n_{00}	n_{01}	n_{0+}	True class	0	N_{00}	N_{01}	N_{0+}
	1	n_{10}	n_{11}	n_{1+}		1	N_{10}	N_{11}	N_{1+}
	Tot	n_{+0}	n_{+1}	n		Tot	N_{+0}	N_{+1}	N

in Section 3, the decision boundaries are numerically derived, indicating under which conditions each of the estimators has the lowest MSE. Finally, in Section 4, we draw our main conclusion and discuss directions for future research.

2 Methods

In this section, five estimators for the base rate parameter α are formally introduced for the binary classification problem. This parameter represents the proportion of objects labeled as class 1 in the unlabeled dataset. Many of these estimators have been proposed decades ago; see [9] for an extensive discussion. We summarize the formulas for bias and variance that can be found in the literature and complement them with our own derivations.

In order to compute new estimates, some information is needed on the specificity and sensitivity of the model. Moreover, there is no need to make corrections if the algorithm is perfect, so we assume that there is a non-zero probability that an object of class i is classified as class $j \neq i$. Sensitivity is defined as the probability that the algorithm predicts an object of class 0 correctly and is written as p_{00} . Specificity is defined as the probability that the algorithm predicts an object of class 1 correctly and is written as p_{11} . It is therefore assumed that each object of class i has the same probability of being classified correctly. These values can be summarized in a matrix \mathbf{P} :

$$\mathbf{P} = \begin{pmatrix} p_{00} & 1 - p_{00} \\ 1 - p_{11} & p_{11} \end{pmatrix}. \quad (1)$$

Unfortunately, the classification probabilities are unknown in practice. It seems reasonable to assume that the algorithm performs better than guessing, and therefore, p_{00} and p_{11} are assumed to be between 0.5 and 1. In practice, the classification probabilities can be estimated with a test dataset, see Table 1. Assuming that the test data are a simple random sample, we can estimate the sensitivity and specificity by: $\hat{p}_{00} = n_{00}/n_{0+}$ and $\hat{p}_{11} = n_{11}/n_{1+}$. The true sensitivity and specificity can be defined similarly from the (unknown) unlabeled dataset (right-hand panel in Table 1). The true base rate parameter α can be computed as N_{1+}/N . The ratio between the rows of the unlabeled dataset is therefore fixed. On the other hand, the specificity and the sensitivity cannot

be calculated immediately from the theoretical table with the unlabeled data, because the rows are drawn from binomial distributions and are therefore random. The sensitivity (p_{00}) is the expected value of N_{00} divided by N_{0+} and the specificity (p_{11}) is the expected value of N_{11} divided by N_{1+} .

One of the restrictions of the study is that we assume that the test set is much smaller than the unlabeled dataset (i.e. $n \ll N$). This makes it possible to assume that the sample counts in the test set follow binomial distributions given the unlabeled dataset and makes it assumable that the estimator for \mathbf{P} from the test set is distributed independently of an estimator for α based on the predicted classes for the unlabeled dataset.

2.1 Baseline estimator - random sample

The baseline estimator for α is the proportion of data points in the test dataset for which the observed class label is equal to 1. The baseline estimator will be denoted by $\hat{\alpha}_a$. Under the assumptions discussed above, it is immediate that $\hat{\alpha}_a$ is an unbiased estimator for α , i.e.:

$$B[\hat{\alpha}_a] = 0. \quad (2)$$

Since we have assumed that the size n of the test dataset is much smaller than the size N of the population data, we may approximate the distribution of $n\hat{\alpha}_a$ by a binomial distribution with success probability α . The variance, and hence the MSE, of $\hat{\alpha}_a$ is then given by

$$MSE[\hat{\alpha}_a] = V[\hat{\alpha}_a] = \frac{\alpha(1-\alpha)}{n}. \quad (3)$$

This MSE will serve as the baseline value for the other estimators we discuss.

2.2 Classify and count

When applying a trained machine learning algorithm on new data, we may simply count the number of data points for which the predicted class equals 1. The resulting estimator for α , which we will denote by $\hat{\alpha}^*$, is referred to as the 'classify-and-count' estimator, see [4]. In general, the classify-and-count estimator is (strongly) biased, and has almost zero variance. More specifically,

$$E[\hat{\alpha}^*] = \alpha p_{11} + (1-\alpha)(1-p_{00}), \quad (4)$$

and hence

$$B[\hat{\alpha}^*] = \alpha(p_{11}-1) + (1-\alpha)(1-p_{00}), \quad (5)$$

which is zero only if the point (p_{00}, p_{11}) lies on the line through $(1-\alpha, \alpha)$ and $(1, 1)$ in \mathbb{R}^2 , as shown in [14]. The variance of the classify-and-count estimator is derived in [2] and equals

$$V[\hat{\alpha}^*] = \frac{\alpha p_{11}(1-p_{11}) + (1-\alpha)p_{00}(1-p_{00})}{N}. \quad (6)$$

If the population size N is large, the variance of $\hat{\alpha}^*$ is low. In some literature, this low variance is misinterpreted as high accuracy, by claiming intuitively that the large size of the dataset implies that the noise cancels out (cf. [13]). However, the nonzero bias is neglected in such arguments. Therefore, we are interested in the MSE because it considers both bias and variance. It equals

$$MSE[\hat{\alpha}^*] = \left(\alpha(p_{11} - 1) + (1 - \alpha)(1 - p_{00}) \right)^2 + O\left(\frac{1}{N}\right). \quad (7)$$

Here and below, the notation $O(x)$ indicates a remainder term that is always contained inside an interval $(-Cx, Cx)$ for some constant $C > 0$; see, e.g., [8]. Observe how, in general, the MSE does not converge to 0 as N tends to ∞ .

2.3 Subtracting estimated bias

Knowing that the classify-and-count estimator $\hat{\alpha}^*$ is biased (see (5)), we may attempt to estimate that bias and subtract it from $\hat{\alpha}^*$. As briefly mentioned in [14], we may estimate that bias by the plug-in estimator, that is, we substitute the unknown quantities in Equation (5) by their estimates. More precisely, the bias is estimated as

$$\hat{B}[\hat{\alpha}^*] = \hat{\alpha}^*(\hat{p}_{00} + \hat{p}_{11} - 2) + (1 - \hat{p}_{00}), \quad (8)$$

in which the estimators \hat{p}_{00} and \hat{p}_{11} are based on the test dataset. The resulting estimator $\hat{\alpha}_b$ for α equals

$$\hat{\alpha}_b = \hat{\alpha}^* - \hat{B}[\hat{\alpha}^*] = \hat{\alpha}^*(3 - \hat{p}_{00} - \hat{p}_{11}) - (1 - \hat{p}_{00}). \quad (9)$$

To the best of our knowledge, the bias and variance of the estimator $\hat{\alpha}_b$ have not been published in the scientific literature. Therefore, we have derived both, up to terms of order $1/n^2$, yielding the following result.

Theorem 1. *The bias of $\hat{\alpha}_b$ as estimator for α is given by*

$$B[\hat{\alpha}_b] = (1 - p_{00})(2 - p_{00} - p_{11}) - \alpha(p_{00} + p_{11} - 2)^2. \quad (10)$$

The variance of $\hat{\alpha}_b$ equals

$$\begin{aligned} V[\hat{\alpha}_b] &= \frac{[\alpha(p_{00} + p_{11} - 1) - p_{00}]^2 p_{00}(1 - p_{00})}{n(1 - \alpha)} \left(1 + \frac{\alpha}{n(1 - \alpha)} \right) \\ &\quad + \frac{[\alpha(p_{00} + p_{11} - 1) + (1 - p_{00})]^2 p_{11}(1 - p_{11})}{n\alpha} \left(1 + \frac{1 - \alpha}{n\alpha} \right) \\ &\quad + O\left(\max\left[\frac{1}{n^3}, \frac{1}{N}\right]\right). \end{aligned} \quad (11)$$

Proof. See the Appendix.

In particular, Theorem 1 implies that $B[\hat{\alpha}_b] = (2 - p_{00} - p_{11})B[\hat{\alpha}^*]$, compare Equations (10) and (5). Hence, $|B[\hat{\alpha}_b]| \leq |B[\hat{\alpha}^*]|$, because $1 < p_{00} + p_{11} < 2$.

2.4 Misclassification probabilities

Let \mathbf{P} be the row-normalized confusion matrix of the machine learning algorithm that we have trained, as defined in (1). That is, entry p_{ij} is the probability that the algorithm predicts class j for a data point that belongs to class i . The probabilities p_{ij} are referred to as misclassification probabilities. In the binary setting, we write α for the column vector $(1 - \alpha, \alpha)^T$ (similarly for $\hat{\alpha}^*$). Under the assumption that the probabilities p_{ij} are identical for each data point, we obtain the expression $E[\hat{\alpha}^*] = \mathbf{P}^T \alpha$. If the true values of all entries p_{ij} of \mathbf{P} were known and if $p_{00} + p_{11} \neq 1$, then $\hat{\alpha}_p = (\mathbf{P}^T)^{-1} \hat{\alpha}^*$ would be an unbiased estimator for α . Using the plug-in estimator $\hat{\mathbf{P}}$ for \mathbf{P} , estimated on the test set, the following estimator for α is obtained:

$$\hat{\alpha}_p = \frac{\hat{\alpha}^* + \hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}. \quad (12)$$

It is known that the estimator $\hat{\alpha}_p$ is consistent (asymptotically unbiased) for α , see [1]. In [5], the variance of this estimator is analysed for an arbitrary number of classes. For the binary case, a simple analytic expression for the bias and variance of $\hat{\alpha}_p$ for finite datasets has not been given, as far as we know. Therefore, we have derived the bias and variance for finite datasets, yielding the following result.

Theorem 2. *The bias of $\hat{\alpha}_p$ as estimator for α is given by*

$$B[\hat{\alpha}_p] = \frac{p_{00} - p_{11}}{n(p_{00} + p_{11} - 1)} + O\left(\frac{1}{n^2}\right). \quad (13)$$

The variance of $\hat{\alpha}_p$ is given by

$$\begin{aligned} V[\hat{\alpha}_p] = & \frac{(1 - \alpha)p_{00}(1 - p_{00}) \left[1 + \frac{\alpha}{n(1 - \alpha)}\right] + \alpha p_{11}(1 - p_{11}) \left[1 + \frac{1 - \alpha}{n\alpha}\right]}{n(p_{00} + p_{11} - 1)^2} \\ & + O\left(\max\left[\frac{1}{n^2}, \frac{1}{N}\right]\right). \end{aligned} \quad (14)$$

Proof. See the Appendix.

2.5 Calibration probabilities

Let \mathbf{C} be the column-normalized confusion matrix of the machine learning algorithm that we have trained. That is, entry c_{ij} is the probability that the true class of a data point is j given that the algorithm has predicted class i . The probabilities c_{ij} are referred to as calibration probabilities [9]. The first element of the vector $\mathbf{C}\hat{\alpha}^*$ is an unbiased estimator for α , if \mathbf{C} is known.

Using the plug-in estimator $\hat{\mathbf{C}}$ for \mathbf{C} , which is estimated on the test dataset analogously to $\hat{\mathbf{P}}$, the following estimator $\hat{\alpha}_c$ for α is obtained:

$$\hat{\alpha}_c = \hat{\alpha}^* \frac{n_{11}}{n_{+1}} + (1 - \hat{\alpha}^*) \frac{n_{10}}{n_{+0}}, \quad (15)$$

in which each n_{ij} and n_{+j} should be considered as random variables. It has been shown that $\hat{\alpha}_c$ is a consistent estimator for α [1]. Under the assumptions we have made in this paper, it can be shown that $\hat{\alpha}_c$ is in fact an unbiased estimator for α . To the best of our knowledge, we are also the first to give an approximation (up to terms of order $1/n^2$) of the variance of $\hat{\alpha}_c$. Both results are summarized in the following theorem.

Theorem 3. *The calibration estimator $\hat{\alpha}_c$ is an unbiased estimator for α :*

$$B[\hat{\alpha}_c] = 0. \quad (16)$$

The variance of $\hat{\alpha}_c$ is equal to the following expression:

$$\begin{aligned} V(\hat{\alpha}_c) = & \left[\frac{(1-\alpha)(1-p_{00}) + \alpha p_{11}}{n} + \frac{(1-\alpha)p_{00} + \alpha(1-p_{11})}{n^2} \right] \\ & \times \left[\frac{\alpha p_{11}}{(1-\alpha)(1-p_{00}) + \alpha p_{11}} \left(1 - \frac{\alpha p_{11}}{(1-\alpha)(1-p_{00}) + \alpha p_{11}} \right) \right] \\ & + \left[\frac{(1-\alpha)p_{00} + \alpha(1-p_{11})}{n} + \frac{(1-\alpha)(1-p_{00}) + \alpha p_{11}}{n^2} \right] \\ & \times \left[\frac{(1-\alpha)p_{00}}{(1-\alpha)p_{00} + \alpha(1-p_{11})} \left(1 - \frac{(1-\alpha)p_{00}}{(1-\alpha)p_{00} + \alpha(1-p_{11})} \right) \right] \\ & + O\left(\max\left[\frac{1}{n^3}, \frac{1}{Nn}\right]\right). \end{aligned} \quad (17)$$

Proof. See the Appendix.

Hereby, the overview of the five estimators for α is complete. The expressions that we have derived for the bias and variance of these five estimators will now be used to compare the (root) mean squared error of the five estimators, both theoretically as well as by means of simulation studies.

3 Results

The aim of this section is to derive empirically which of the five estimators of α that we presented in Section 2 has the lowest MSE, and under which conditions. For a given population size N , the MSE of each estimator depends on four parameters (i.e., $\alpha, p_{00}, p_{11}, n$), so visualizations would have to be 5-dimensional. To reduce dimensions, we will first present a simulation study in which all four parameters are fixed. For the fixed parameter setting, the sampling distributions of the estimators are compared using boxplots. Second, we will fix several values of α and n and use plots to compare the MSE of the estimators for varying p_{00} and p_{11} . The latter analysis will already be sufficient in order to reach a final conclusion on which estimator has the lowest MSE.^{||}

^{||}The results in this section have been obtained using the statistical software R. All visualizations have been implemented in a Shiny dashboard, which in addition includes interactive 3D-plots of the RMSE surface for each of the estimators. The code can be retrieved from <https://github.com/kevinkloos/Misclassification-Bias>.

3.1 Sampling distributions of the estimators

Here, we present two simple simulation studies to gain some intuition for the difference in the sampling distributions of the five estimators. In the first simulation study, we consider a class-balanced dataset, that is, $\alpha = 0.5$, with a small test dataset of size $n = 1000$, a large population dataset $N = 3 \times 10^6$ and a rather poor classifier having classification probabilities $p_{00} = 0.6$ and $p_{11} = 0.7$. We deliberately choose $p_{00} \neq p_{11}$, as otherwise the classify-and-count estimator $\hat{\alpha}^*$ would be unbiased: (p_{00}, p_{11}) would be on the line between $(1 - \alpha, \alpha)$ and $(1, 1)$, see also Equation (5).

Table 2 summarizes the bias, variance and root mean squared error (RMSE), computed using the analytic approximations presented in Section 2. The classify-and-count estimator is highly biased and therefore it has a high RMSE, despite having the lowest variance of all estimators. The RMSE of the classify-and-count estimator can indeed be improved by subtracting an estimate of the bias ($\hat{\alpha}_b$). The subtraction reduces the absolute bias and only slightly increases the variance. A further bias reduction is obtained by the misclassification estimator $\hat{\alpha}_p$. However, inverting the row-normalized confusion matrix \mathbf{P} (that is, the misclassification probabilities) for values of p_{00} and p_{11} close to $p_{00} + p_{11} = 1$ significantly increases the variance of the estimator, leading to the highest RMSE of all estimators considered. Finally, the calibration estimator $\hat{\alpha}_c$ is unbiased and has the lowest variance among the estimators that make use of the test dataset. In particular, note that the variance is also lower than that of the baseline estimator. In this example, the estimator based on the calibration probabilities has the lowest RMSE, and it is the only estimator with a lower RMSE than the baseline estimator $\hat{\alpha}_a$. To gain insight in the sampling distribution of

Table 2: A comparison of the bias, variance and RMSE of each of the five estimators for α , where $\alpha = 0.5$, $p_{00} = 0.6$, $p_{11} = 0.7$, $n = 1000$ and $N = 3 \times 10^6$.

<i>Estimator</i>	<i>Symbol</i>	Bias $\times 10^{-2}$	Variance $\times 10^{-4}$	RMSE $\times 10^{-2}$
Baseline	$\hat{\alpha}_a$	0.000	2.500	1.581
Classify-and-count	$\hat{\alpha}^*$	5.000	0.000	5.000
Subtracted-bias	$\hat{\alpha}_b$	-3.500	2.244	3.807
Misclassification	$\hat{\alpha}_p$	-0.033	25.025	5.003
Calibration	$\hat{\alpha}_c$	0.000	2.275	1.508

the estimators, in addition to the metrics presented in Table 2, we simulated a large number $R = 10000$ of confusion matrices for datasets of size $n = 1000$. Each confusion matrix was created as follows. First, take a random draw from a $\text{Bin}(n, \alpha)$ -distribution, resulting in a number n_{1+} . Then, take a random draw

from a $\text{Bin}(n_{1+}, p_{11})$ -distribution (i.e., the number of true positives) and a random draw from a $\text{Bin}(n - n_{1+}, p_{00})$ -distribution (i.e., the number of true negatives). These three consecutive draws precisely give the number of true and false positives and negatives needed to fill a confusion matrix. Each confusion matrix can be used to compute the five estimators. Repeating this procedure $R = 10000$ times gave rise to the sampling distributions of the five estimators as presented in Figure 1. It nicely visualizes the bias and variance of the five estimators, supporting the results in Table 2. In addition, it shows that the variance of the classify-and-count estimator $\hat{\alpha}^*$ and the subtracted-bias estimator $\hat{\alpha}_b$ cannot be used to obtain reliable confidence intervals for α . In the second

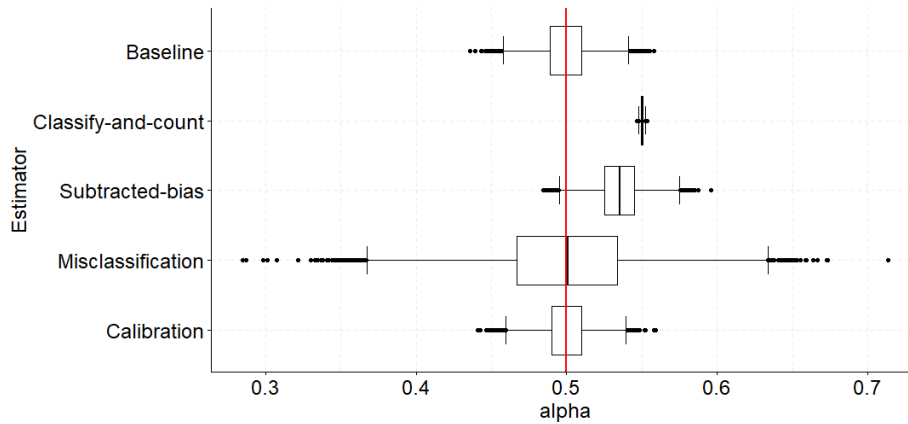


Fig. 1: The boxplots show the sampling distribution of the estimators for α , where $\alpha = 0.5$, $p_{00} = 0.6$, $p_{11} = 0.7$ and $n = 1000$. The true value of α is highlighted by a vertical line.

simulation study, we consider a highly imbalanced dataset, namely $\alpha = 0.98$. We again assume that the available test dataset has size $n = 1000$, but we assume a classifier having classification probabilities $p_{00} = 0.94$ and $p_{11} = 0.97$. Table 3 summarizes the bias, variance and RMSE of each of the estimators and Figure 2 shows the sampling distributions of each of the estimators. It can be noticed that subtracted-bias estimator and the misclassification estimator both have estimates of α that exceed 1. It is obvious that such values cannot occur in the population. For the method with the misclassification probabilities, this effect gets stronger when $p_{00} + p_{11}$ gets closer to 1. Furthermore, the baseline estimator performs well compared to the other estimators when the dataset is highly imbalanced: its RMSE is slightly higher than the RMSE of the method with calibration probabilities and much lower than the method with the misclassification probabilities. Finally, it can be shown that the classify-and-count estimator is highly biased, even though p_{00} and p_{11} are both fairly close to 1.

Table 3: A comparison of the bias, variance and RMSE of each of the five estimators for α , where $\alpha = 0.98$, $p_{00} = 0.94$, $p_{11} = 0.97$, $n = 1000$ and $N = 3 \times 10^6$.

<i>Method</i>	<i>Symbol</i>	Bias $\times 10^{-2}$	Variance $\times 10^{-5}$	RMSE $\times 10^{-3}$
Baseline	$\hat{\alpha}_a$	0.000	1.960	4.427
Classify-and-count	$\hat{\alpha}^*$	-2.820	0.000	28.200
Subtracted-bias	$\hat{\alpha}_b$	0.254	3.377	6.342
Misclassification	$\hat{\alpha}_p$	-0.003	3.587	5.989
Calibration	$\hat{\alpha}_c$	0.000	1.289	3.591

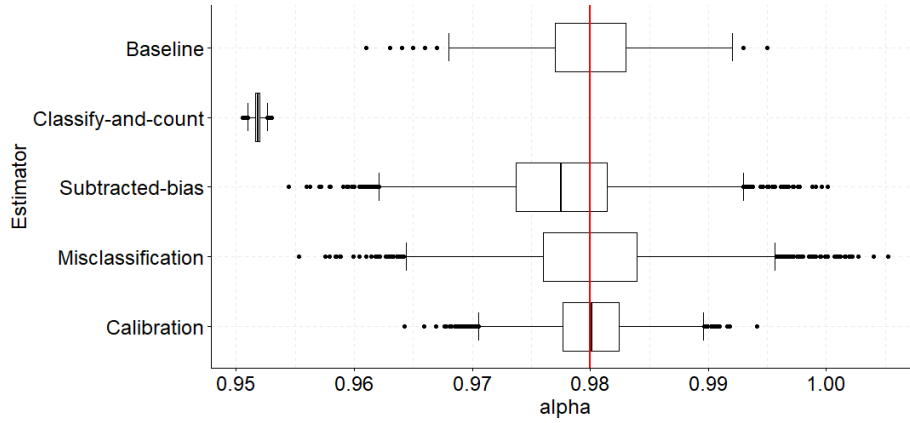


Fig. 2: The boxplots show the sampling distribution of the estimators for α , where $\alpha = 0.98$, $p_{00} = 0.94$, $p_{11} = 0.97$, $n = 1000$ and $N = 3 \times 10^6$. The true value of α is highlighted by a vertical line.

3.2 Finding the optimal estimator

The aim of this subsection is to find the optimal estimator, i.e., the estimator with the lowest RMSE, for every combination of values of the parameters α , p_{00} , p_{11} and n . First, suppose that (p_{00}, p_{11}) is close to the line in the plane through the points $(1 - \alpha, \alpha)$ and $(1, 1)$. As noted before, it implies that the classify-and-count estimator $\hat{\alpha}^*$ has low bias. Consequently, the subtracted-bias estimator $\hat{\alpha}_b$ has low bias as well. Thus, these two estimators will have the lowest RMSE in the described region, whose size decreases as n increases. Figure 3 visualizes the described region for $\alpha = 0.2$ and two different values of n . We remark that the biased estimators $\hat{\alpha}^*$ and $\hat{\alpha}_b$ perform worse (relative to the other estimators) when the sample size n of the test dataset increases. The biased correction methods perform well when the classification probabilities are high for the largest group.

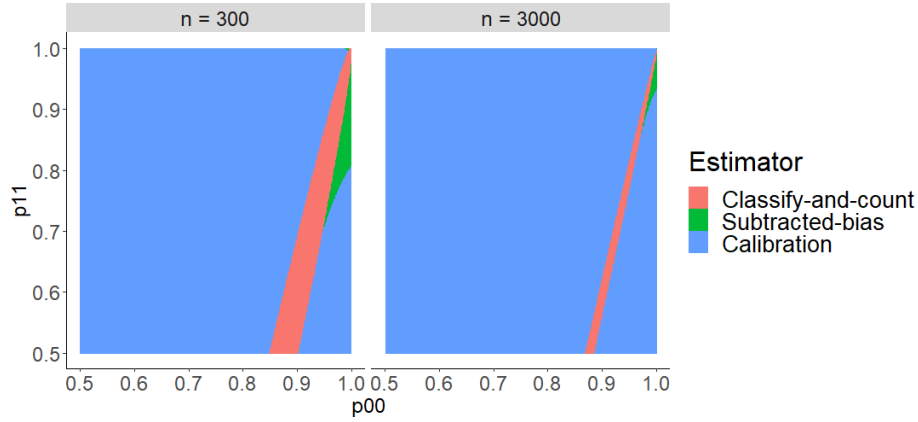


Fig. 3: For each coordinate (p_{00}, p_{11}) , the depicted color indicates which estimator has the lowest RMSE, considering only the classify-and-count estimator (red), the subtracted-bias estimator (green) and the calibration estimator (blue). In the left panel, we have set $\alpha = 0.2$ and $n = 300$, whereas $\alpha = 0.2$ and $n = 3000$ in the right panel. The red and green regions are smaller in the left panel, as the variance of the calibration estimator is decreasing in n , while the bias of the classify-and-count estimator and of the subtracted-bias estimator do not depend on n .

As we have seen in both Table 2 and Table 3, the calibration estimator $\hat{\alpha}_c$ competes with the baseline estimator in having the lowest RMSE. In general, the calibration estimator will have lower RMSE if the classification probabilities p_{00} and p_{11} are higher, while the baseline estimator does not depend on these classification probabilities. In a neighbourhood of $p_{00} = p_{11} = 0.5$, the baseline estimator will always have lower RMSE than the calibration estimator. However, for every α and n , there must exist a curve in the (p_{00}, p_{11}) -plane beyond which the calibration estimator will have lower RMSE than the baseline estimator. The left-hand panels in Figure 4 show this curve for $\alpha = 0.2$ and two different values of n . For larger values of n , the curve where the calibration estimator performs better than the baseline estimator gets closer to $p_{00} = p_{11} = 0.5$ and therefore covers a larger area in the (p_{00}, p_{11}) -plane.

Table 2 and Table 3 have shown that the misclassification estimator only performs well if p_{00} and p_{11} are high, which is confirmed by the expression of the bias and variance: both have a singularity at $p_{00} + p_{11} = 1$, see Equations (13) and (14). The right-hand panels in Figure 4 show, for $\alpha = 0.2$ and two different values of n , the curve in the (p_{00}, p_{11}) -plane beyond which the misclassification estimator has lower RMSE than the baseline estimator. Observe that an increase in the size n of the test dataset does not have much impact on the position of the curve. The reason is that the misclassification estimator has a singularity at $p_{00} = p_{11} = 0.5$. The shape of the curve also depends on the value of α .

If $\alpha = 0.8$ instead of 0.2, the curves are line-symmetric in the line $p_{00} = p_{11}$. The curve is also line symmetric in $p_{00} = p_{11}$ for $\alpha = 0.5$. The area where the misclassification estimator performs better than the baseline estimator decreases when α gets closer towards 0 or 1. The main reason why this happens is that the variance of the baseline estimator decreases fast when α gets closer towards 0 or 1. Thus, the baseline estimator performs better than the misclassification estimator either if the classifier performs badly or if the classification probability of the largest group is low.

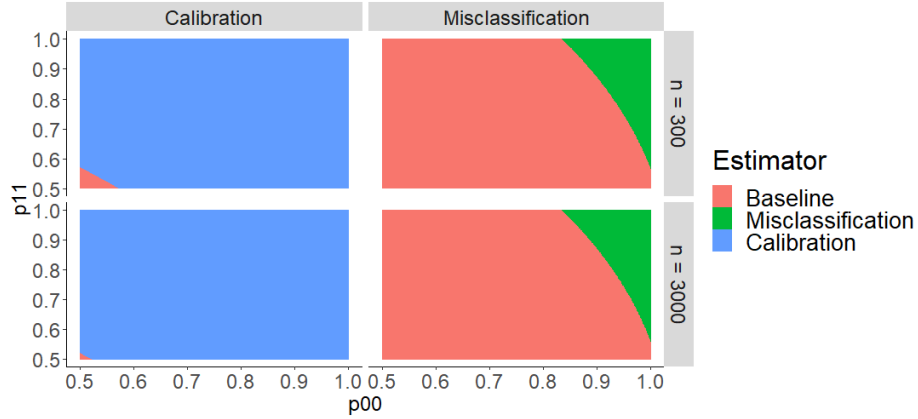


Fig. 4: For each coordinate (p_{00}, p_{11}) , the depicted color indicates which estimate has the lowest RMSE, considering only the baseline estimator (red), the calibration estimator (blue) and the misclassification estimator (green). The top-row panels consider $\alpha = 0.2$ and $n = 300$, while the bottom-row panels consider $\alpha = 0.2$ and $n = 3000$.

It remains to compare the calibration estimator and the misclassification estimator for high values of p_{00} and p_{11} . In Theorem 4 it is proven that, for all possible combinations of α and sufficiently large n , the MSE of the calibration estimator is consistently lower than that of the misclassification estimator.

Theorem 4. *Let $\widetilde{MSE}[\hat{\alpha}_p]$ and $\widetilde{MSE}[\hat{\alpha}_c]$ denote the approximate mean squared errors, up to terms of order $1/n$, of the misclassification estimator and the calibration estimator, respectively. It holds that:*

$$\widetilde{MSE}[\hat{\alpha}_p] - \widetilde{MSE}[\hat{\alpha}_c] = \frac{\left((1 - \alpha)p_{00}(1 - p_{00}) + \alpha p_{11}(1 - p_{11})\right)^2}{(p_{00} + p_{11} - 1)^2 \beta (1 - \beta)}, \quad (18)$$

in which $\beta := (1 - \alpha)(1 - p_{00}) + \alpha p_{11}$.

Proof. See the Appendix.

Thus, neglecting terms of order $1/n^2$ and higher, the result implies that the calibration estimator has a lower mean squared error than the misclassification estimator, with equality if and only if $p_{00} = p_{11} = 1$. (Note that $0 < \beta < 1$.)

We do remark that the difference in MSE is large in particular for values of p_{00} and p_{11} close to $\frac{1}{2}$. More specifically, it diverges when $p_{00} + p_{11} \rightarrow 1$. It is the result of the misclassification estimator having a singularity at $p_{00} + p_{11} = 1$ (see Equation (14)), while the variance of the calibration estimator is bounded. An unpleasant consequence of the singularity at $p_{00} + p_{11} = 1$ is that, for fixed n and α , the probability that $\hat{\alpha}_p$ takes values outside the interval $[0, 1]$ increases as $p_{00} + p_{11} \rightarrow 1$; see [12] for a discussion and a possible solution.

4 Conclusion and Discussion

In this paper, we have studied the effect of classification errors on five estimators of the base rate parameter α that are obtained from machine learning algorithms. In general, a straightforward classify-and-count estimator will lead to biased estimates and some form of bias correction should be considered. As reducing bias might increase variance, we evaluated the (root) mean squared error (MSE) of the five estimators, both theoretically as well as numerically.

From our results we may draw the following main (three-part) conclusion regarding which estimator for α has lowest mean squared error. First, when dealing with small test datasets and rather poor algorithms, that is p_{00} and p_{11} both close to 0.5, the baseline estimator $\hat{\alpha}_a$ has the lowest MSE. Second, when dealing with algorithms for which the classification probabilities p_{00} and p_{11} are in a small neighbourhood around the line $(p_{11} - 1)\alpha + (1 - p_{00})(1 - \alpha) = 0$ in the (p_{00}, p_{11}) -plane, the classify-and-count estimator and the subtracted-bias estimator will have the lowest MSE. As the size of the test dataset increases, the size of that neighbourhood decreases. Third, in any other situation, the calibration estimator will have the lowest MSE. In practice, the test dataset will have to be used to determine which of the three scenarios applies to the data and the algorithm at hand. It is an additional estimation problem that we have not discussed in this paper.

We would like to close the paper by pointing out three interesting directions for future research. First, the results could be generalized to multi-class classification problems. The theoretical derivations of the bias and variance are more complicated and involve matrix-vector notation, but the proof strategy is similar. However, it is more challenging to compare the MSE of the five estimators visually in the multi-class case.

Second, the assumptions that we have made could be relaxed. In particular, a trained and implemented machine learning model is, in practice, often used over a longer period of time. A shift in the base rate parameter α , also known as concept drift [16], is then inevitable. Consequently, we may no longer assume that the conditional distribution of the class label given the features in the test dataset is similar to that in the population. It implies that the calibration

estimator is no longer unbiased, which might have a significant effect on our main conclusion.

Third and finally, a combination of estimators might have a lower MSE than that of the individual estimators separately. Therefore, it might be interesting to study different methods of model averaging applied to the problem of misclassification bias. It could be fruitful especially when the assumptions that we have made are relaxed.

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Appendix

This appendix contains the proofs of the theorems presented in the paper entitled "Comparing Correction Methods for Misclassification Bias". Recall that we have assumed a population of size N in which a fraction $\alpha := N_{1+}/N$ belongs to the class of interest, referred to as the class labelled as 1. We assume that a binary classification algorithm has been trained that correctly classifies a data point that belongs to class $i \in \{0, 1\}$ with probability $p_{ii} > 0.5$, independently across all data points. In addition, we assume that a test set of size $n \ll N$ is available and that it can be considered a simple random sample from the population. The classification probabilities p_{00} and p_{11} are estimated on that test set as described in Section 2. Finally, we assume that the classify-and-count estimator $\hat{\alpha}^*$ is distributed independently of \hat{p}_{00} and \hat{p}_{11} , which is reasonable (at least as an approximation) when $n \ll N$.

It may be noted that the estimated probabilities \hat{p}_{11} and \hat{p}_{00} defined in Section 2 cannot be computed if $n_{1+} = 0$ or $n_{0+} = 0$. Similarly, the calibration probabilities c_{11} and c_{00} cannot be estimated if $n_{+1} = 0$ or $n_{+0} = 0$. We assume here that these events occur with negligible probability. This will be true when n is sufficiently large so that $n\alpha \gg 1$ and $n(1 - \alpha) \gg 1$.

Preliminaries

Many of the proofs presented in this appendix rely on the following two mathematical results. First, we will use univariate and bivariate Taylor series to approximate the expectation of non-linear functions of random variables. That is, to estimate $E[f(X)]$ and $E[g(X, Y)]$ for sufficiently differentiable functions f and g , we will insert the Taylor series for f and g at $x_0 = E[X]$ and $y_0 = E[Y]$ up to terms of order 2 and utilize the linearity of the expectation. Second, we will use the following conditional variance decomposition for the variance of a random variable X :

$$V(X) = E[V(X | Y)] + V(E[X | Y]). \quad (19)$$

The conditional variance decomposition follows from the tower property of conditional expectations [8]. Before we prove the theorems presented in the paper, we begin by proving the following lemma.

Lemma 1. *The variance of the estimator \hat{p}_{11} for p_{11} estimated on the test set is given by*

$$V(\hat{p}_{11}) = \frac{p_{11}(1 - p_{11})}{n\alpha} \left[1 + \frac{1 - \alpha}{n\alpha} \right] + O\left(\frac{1}{n^3}\right). \quad (20)$$

Similarly, the variance of \hat{p}_{00} is given by

$$V(\hat{p}_{00}) = \frac{p_{00}(1 - p_{00})}{n(1 - \alpha)} \left[1 + \frac{\alpha}{n(1 - \alpha)} \right] + O\left(\frac{1}{n^3}\right). \quad (21)$$

Moreover, \hat{p}_{11} and \hat{p}_{00} are uncorrelated: $C(\hat{p}_{11}, \hat{p}_{00}) = 0$.

Proof (of Lemma 1). We approximate the variance of \hat{p}_{00} using the conditional variance decomposition and a second-order Taylor series, as follows:

$$\begin{aligned}
V(\hat{p}_{00}) &= V\left(\frac{n_{00}}{n_{0+}}\right) \\
&= E_{n_{0+}}\left[V\left(\frac{n_{00}}{n_{0+}} \mid n_{0+}\right)\right] + V_{n_{0+}}\left[E\left(\frac{n_{00}}{n_{0+}} \mid n_{0+}\right)\right] \\
&= E_{n_{0+}}\left[\frac{1}{n_{0+}^2}V(n_{00} \mid n_{0+})\right] + V_{n_{0+}}\left[\frac{1}{n_{0+}}E(n_{00} \mid n_{0+})\right] \\
&= E_{n_{0+}}\left[\frac{n_{0+}p_{00}(1-p_{00})}{n_{0+}^2}\right] + V_{n_{0+}}\left[\frac{n_{0+}p_{00}}{n_{0+}}\right] \\
&= E_{n_{0+}}\left[\frac{1}{n_{0+}}\right]p_{00}(1-p_{00}) \\
&= \left[\frac{1}{E[n_{0+}]} + \frac{1}{2}\frac{2}{E[n_{0+}]^3} \times V[n_{0+}]\right]p_{00}(1-p_{00}) + O\left(\frac{1}{n^3}\right) \\
&= \frac{p_{00}(1-p_{00})}{E[n_{0+}]} \left[1 + \frac{V[n_{0+}]}{E[n_{0+}]^2}\right] + O\left(\frac{1}{n^3}\right) \\
&= \frac{p_{00}(1-p_{00})}{n(1-\alpha)} \left[1 + \frac{\alpha}{n(1-\alpha)}\right] + O\left(\frac{1}{n^3}\right).
\end{aligned}$$

The variance of \hat{p}_{11} is approximated in the exact same way.

Finally, to evaluate $C(\hat{p}_{11}, \hat{p}_{00})$ we use the analogue of (19) for covariances:

$$\begin{aligned}
C(\hat{p}_{11}, \hat{p}_{00}) &= C\left(\frac{n_{11}}{n_{1+}}, \frac{n_{00}}{n_{0+}}\right) \\
&= E_{n_{1+}, n_{0+}}\left[C\left(\frac{n_{11}}{n_{1+}}, \frac{n_{00}}{n_{0+}} \mid n_{1+}, n_{0+}\right)\right] \\
&\quad + C_{n_{1+}, n_{0+}}\left[E\left(\frac{n_{11}}{n_{1+}} \mid n_{1+}, n_{0+}\right), E\left(\frac{n_{00}}{n_{0+}} \mid n_{1+}, n_{0+}\right)\right] \\
&= E_{n_{1+}, n_{0+}}\left[\frac{1}{n_{1+}n_{0+}}C(n_{11}, n_{00} \mid n_{1+}, n_{0+})\right] \\
&\quad + C_{n_{1+}, n_{0+}}\left[\frac{1}{n_{1+}}E(n_{11} \mid n_{1+}), \frac{1}{n_{0+}}E(n_{00} \mid n_{0+})\right].
\end{aligned}$$

The second term is zero as before. The first term also vanishes because, conditional on the row totals n_{1+} and n_{0+} , the counts n_{11} and n_{00} follow independent binomial distributions, so $C(n_{11}, n_{00} \mid n_{1+}, n_{0+}) = 0$.

Note: in the remainder of this appendix, we will not add explicit subscripts to expectations and variances when their meaning is unambiguous.

Subtracted-bias estimator

We will now prove the bias and variance approximations for the subtracted-bias estimator $\hat{\alpha}_b$ that was defined in Equation (9).

Proof (of Theorem 1). The bias of $\hat{\alpha}_b$ is given by

$$\begin{aligned}
B(\hat{\alpha}_b) &= E \left[\hat{\alpha}^* - \hat{B}[\hat{\alpha}^*] \right] - \alpha \\
&= E[\hat{\alpha}^* - \alpha] - E \left[\hat{B}[\hat{\alpha}^*] \right] \\
&= B[\hat{\alpha}^*] - E \left[\hat{B}[\hat{\alpha}^*] \right] \\
&= [\alpha(p_{00} + p_{11} - 2) + (1 - p_{00})] - E[\hat{\alpha}^*(\hat{p}_{00} + \hat{p}_{11} - 2) + (1 - \hat{p}_{00})].
\end{aligned}$$

Because $\hat{\alpha}^*$ and $(\hat{p}_{00} + \hat{p}_{11} - 2)$ are assumed to be independent, the expectation of their product equals the product of their expectations:

$$\begin{aligned}
B(\hat{\alpha}_b) &= \alpha(p_{00} + p_{11} - 2) + (1 - p_{00}) - E[\hat{\alpha}^*](p_{00} + p_{11} - 2) - (1 - p_{00}) \\
&= (\alpha - E[\hat{\alpha}^*])(p_{00} + p_{11} - 2) \\
&= B[\hat{\alpha}^*](2 - p_{00} - p_{11}) \\
&= (1 - p_{00})(2 - p_{00} - p_{11}) - \alpha(p_{00} + p_{11} - 2)^2.
\end{aligned}$$

This proves the formula for the bias of $\hat{\alpha}_b$ as estimator for α . To approximate the variance of $\hat{\alpha}_b$, we apply the conditional variance decomposition (19) conditional on $\hat{\alpha}^*$ and look at the two resulting terms separately. First, consider the expectation of the conditional variance:

$$\begin{aligned}
E[V(\hat{\alpha}_b \mid \hat{\alpha}^*)] &= E[V(\hat{\alpha}^*(3 - \hat{p}_{00} - \hat{p}_{11}) - (1 - \hat{p}_{00}) \mid \hat{\alpha}^*)] \\
&= E[V(\hat{\alpha}^*(3 - \hat{p}_{00} - \hat{p}_{11}) \mid \hat{\alpha}^*) + V(1 - \hat{p}_{00} \mid \hat{\alpha}^*) \\
&\quad - 2C(\hat{\alpha}^*(3 - \hat{p}_{00} - \hat{p}_{11}), 1 - \hat{p}_{00} \mid \hat{\alpha}^*)] \\
&= E[(\hat{\alpha}^*)^2 V(3 - \hat{p}_{00} - \hat{p}_{11} \mid \hat{\alpha}^*) + V(1 - \hat{p}_{00} \mid \hat{\alpha}^*) \\
&\quad - 2\hat{\alpha}^* C(3 - \hat{p}_{00} - \hat{p}_{11}, 1 - \hat{p}_{00} \mid \hat{\alpha}^*)] \\
&= E[(\hat{\alpha}^*)^2 [V(\hat{p}_{00}) + V(\hat{p}_{11})] + V(\hat{p}_{00}) - 2\hat{\alpha}^* V(\hat{p}_{00})] \\
&= E[(\hat{\alpha}^*)^2] [V(\hat{p}_{00}) + V(\hat{p}_{11})] + V(\hat{p}_{00}) - 2E[\hat{\alpha}^*] V(\hat{p}_{00}).
\end{aligned}$$

In the penultimate line, we used that $C(\hat{p}_{11}, \hat{p}_{00}) = 0$. The second moment $E[(\hat{\alpha}^*)^2]$ can be written as $E[\hat{\alpha}^*]^2 + V(\hat{\alpha}^*)$. Because $V(\hat{\alpha}^*)$ is of order $1/N$, it can be neglected compared to $E[\hat{\alpha}^*]^2$, which is of order 1. In particular, we find that the expectation of the conditional variance equals:

$$\begin{aligned}
E[V(\hat{\alpha}_b \mid \hat{\alpha}^*)] &= E[(\hat{\alpha}^*)^2] [V(\hat{p}_{00}) + V(\hat{p}_{11})] + V(\hat{p}_{00}) - 2E[\hat{\alpha}^*] V(\hat{p}_{00}) + O\left(\frac{1}{N}\right) \\
&= V(\hat{p}_{00}) [E[\hat{\alpha}^*] - 1]^2 + V(\hat{p}_{11}) E[\hat{\alpha}^*]^2 + O\left(\frac{1}{N}\right).
\end{aligned}$$

Next, the variance of the conditional expectation can be seen to be equal the following:

$$\begin{aligned}
V[E(\hat{\alpha}_b \mid \hat{\alpha}^*)] &= V[E(\hat{\alpha}^*(3 - \hat{p}_{00} - \hat{p}_{11}) - (1 - \hat{p}_{00}) \mid \hat{\alpha}^*)] \\
&= V[\hat{\alpha}^* E(3 - \hat{p}_{00} - \hat{p}_{11} \mid \hat{\alpha}^*) - E(1 - \hat{p}_{00} \mid \hat{\alpha}^*)] \\
&= V(\hat{\alpha}^*)(3 - p_{00} - p_{11})^2.
\end{aligned}$$

Because $V(\hat{\alpha}^*)$ is of order $1/N$, it can be neglected in the final formula. Furthermore, the variances of \hat{p}_{00} and \hat{p}_{11} can be written out using the result from Lemma 1:

$$\begin{aligned} V(\hat{\alpha}_b) = & \frac{[\alpha(p_{00} + p_{11} - 1) - p_{00}]^2 p_{00}(1 - p_{00})}{n(1 - \alpha)} \left[1 + \frac{\alpha}{n(1 - \alpha)} \right] \\ & + \frac{[\alpha(p_{00} + p_{11} - 1) + (1 - p_{00})]^2 p_{11}(1 - p_{11})}{n\alpha} \left[1 + \frac{1 - \alpha}{n\alpha} \right] \\ & + O\left(\max\left[\frac{1}{n^3}, \frac{1}{N}\right]\right). \end{aligned}$$

This concludes the proof of Theorem 1.

Misclassification estimator

We will now prove the bias and variance approximations for the misclassification estimator $\hat{\alpha}_p$ as defined in Equation (12).

Proof (of Theorem 2). Under the assumption that $\hat{\alpha}^*$ is distributed independently of $(\hat{p}_{00}, \hat{p}_{11})$, it holds that

$$\begin{aligned} E(\hat{\alpha}_p) &= E\left(\frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right) + E\left[E\left(\frac{\hat{\alpha}^*}{\hat{p}_{00} + \hat{p}_{11} - 1} \middle| \hat{\alpha}^*\right)\right] \\ &= E\left(\frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right) + E(\hat{\alpha}^*)E\left(\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right). \end{aligned} \quad (22)$$

$E(\hat{\alpha}^*)$ is known from (4). To evaluate the other two expectations, we use a second-order Taylor series approximation. The first- and second-order partial derivatives of $f(x, y) = 1/(x + y - 1)$ and $g(x, y) = (x - 1)/(x + y - 1) = 1 - [y/(x + y - 1)]$ are given by:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = \frac{-1}{(x + y - 1)^2}, \quad (23)$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial y^2} = \frac{2}{(x + y - 1)^3},$$

$$\frac{\partial g}{\partial x} = \frac{y}{(x + y - 1)^2}, \quad (24)$$

$$\frac{\partial g}{\partial y} = \frac{-(x - 1)}{(x + y - 1)^2}, \quad (25)$$

$$\frac{\partial^2 g}{\partial x^2} = \frac{-2y}{(x + y - 1)^3},$$

$$\frac{\partial^2 g}{\partial y^2} = \frac{2(x - 1)}{(x + y - 1)^3}.$$

Now also using that $C(\hat{p}_{11}, \hat{p}_{00}) = 0$, we obtain for the first expectation:

$$\begin{aligned} E\left(\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right) &= \frac{1}{p_{00} + p_{11} - 1} + \frac{V(\hat{p}_{00}) + V(\hat{p}_{11})}{(p_{00} + p_{11} - 1)^3} + O(n^{-2}) \\ &= \frac{1}{p_{00} + p_{11} - 1} \left[1 + \frac{\frac{p_{00}(1-p_{00})}{n(1-\alpha)} + \frac{p_{11}(1-p_{11})}{n\alpha}}{(p_{00} + p_{11} - 1)^2} \right] + O(n^{-2}). \end{aligned} \quad (26)$$

Here, we have included only the first term of the approximations to $V(\hat{p}_{00})$ and $V(\hat{p}_{11})$ from Lemma 1, since this suffices to approximate the bias up to terms of order $O(1/n)$. Similarly, for the second expectation we obtain:

$$\begin{aligned} E\left(\frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right) &= \frac{p_{00} - 1}{p_{00} + p_{11} - 1} + \frac{(p_{00} - 1)V(\hat{p}_{11}) - p_{11}V(\hat{p}_{00})}{(p_{00} + p_{11} - 1)^3} + O(n^{-2}) \\ &= \frac{p_{00} - 1}{p_{00} + p_{11} - 1} \left[1 + p_{11} \frac{\frac{1-p_{11}}{n\alpha} + \frac{p_{00}}{n(1-\alpha)}}{(p_{00} + p_{11} - 1)^2} \right] + O(n^{-2}). \end{aligned} \quad (27)$$

Using (22), (4), (26), and (27), we conclude that:

$$\begin{aligned} E(\hat{\alpha}_p) &= \frac{\alpha(p_{00} + p_{11} - 1) - (p_{00} - 1)}{p_{00} + p_{11} - 1} \left[1 + \frac{\frac{p_{00}(1-p_{00})}{n(1-\alpha)} + \frac{p_{11}(1-p_{11})}{n\alpha}}{(p_{00} + p_{11} - 1)^2} \right] \\ &\quad + \frac{p_{00} - 1}{p_{00} + p_{11} - 1} \left[1 + p_{11} \frac{\frac{1-p_{11}}{n\alpha} + \frac{p_{00}}{n(1-\alpha)}}{(p_{00} + p_{11} - 1)^2} \right] + O\left(\frac{1}{n^2}\right). \end{aligned}$$

From this, it follows that an approximation to the bias of $\hat{\alpha}_p$ that is correct up to terms of order $O(1/n)$ is given by:

$$\begin{aligned} B(\hat{\alpha}_p) &= \frac{\alpha(p_{00} + p_{11} - 1) - (p_{00} - 1)}{n(p_{00} + p_{11} - 1)^3} \left[\frac{p_{00}(1-p_{00})}{1-\alpha} + \frac{p_{11}(1-p_{11})}{\alpha} \right] \\ &\quad + \frac{(p_{00} - 1)p_{11}}{n(p_{00} + p_{11} - 1)^3} \left[\frac{1-p_{11}}{\alpha} + \frac{p_{00}}{1-\alpha} \right] + O\left(\frac{1}{n^2}\right). \end{aligned}$$

By expanding the products in this expression and combining similar terms, the expression can be simplified to:

$$B(\hat{\alpha}_p) = \frac{p_{11}(1-p_{11}) - p_{00}(1-p_{00})}{n(p_{00} + p_{11} - 1)^2} + O\left(\frac{1}{n^2}\right).$$

Finally, using the identity $p_{11}(1-p_{11}) - p_{00}(1-p_{00}) = (p_{00} + p_{11} - 1)(p_{00} - p_{11})$, we obtain the required result for $B(\hat{\alpha}_p)$.

To approximate the variance of $\hat{\alpha}_p$, we apply the conditional variance decomposition conditional on $\hat{\alpha}^*$ and look at the two resulting terms separately. First,

consider the variance of the conditional expectation:

$$\begin{aligned}
V[E(\hat{\alpha}_p \mid \hat{\alpha}^*)] &= V\left[E\left(\hat{\alpha}^* \frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1} + \frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1} \mid \hat{\alpha}^*\right)\right] \\
&= V\left[\hat{\alpha}^* \frac{1}{p_{00} + p_{11} - 1}\right] \\
&= \frac{1}{(p_{00} + p_{11} - 1)^2} V[\hat{\alpha}^*] = O\left(\frac{1}{N}\right), \tag{28}
\end{aligned}$$

where in the last line we used (6). Note: the factor $1/(p_{00} + p_{11} - 1)^2$ can become arbitrarily large in the limit $p_{00} + p_{11} \rightarrow 1$. It will be seen below that this same factor also occurs in the lower-order terms of $V(\hat{\alpha}_p)$; hence, the relative contribution of (28) remains negligible even in the limit $p_{00} + p_{11} \rightarrow 1$.

Next, we compute the expectation of the conditional variance.

$$\begin{aligned}
E[V(\hat{\alpha}_p \mid \hat{\alpha}^*)] &= E\left[V\left(\hat{\alpha}^* \frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1} + \frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1} \mid \hat{\alpha}^*\right)\right] \\
&= E\left[V\left(\hat{\alpha}^* \frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1} \mid \hat{\alpha}^*\right) + V\left(\frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1} \mid \hat{\alpha}^*\right) \right. \\
&\quad \left. + 2C\left(\hat{\alpha}^* \frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}, \frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1} \mid \hat{\alpha}^*\right)\right] \\
&= E[(\hat{\alpha}^*)^2] V\left[\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] + V\left[\frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] \\
&\quad + 2E[\hat{\alpha}^*] C\left[\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}, \frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] \\
&= E[\hat{\alpha}^*]^2 \left[1 + O\left(\frac{1}{N}\right)\right] V\left[\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] + V\left[\frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] \\
&\quad + 2E[\hat{\alpha}^*] C\left[\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}, \frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right]. \tag{29}
\end{aligned}$$

To approximate the variance and covariance terms, we use a first-order Taylor series. Using the partial derivatives in (23), (24) and (25), we obtain:

$$\begin{aligned}
V\left[\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] &= \frac{V(\hat{p}_{00}) + V(\hat{p}_{11})}{(p_{00} + p_{11} - 1)^4} + O(n^{-2}) \\
V\left[\frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] &= \frac{V(\hat{p}_{00})(p_{11})^2}{(p_{00} + p_{11} - 1)^4} + \frac{V(\hat{p}_{11})(1 - p_{00})^2}{(p_{00} + p_{11} - 1)^4} + O(n^{-2}) \\
C\left[\frac{1}{\hat{p}_{00} + \hat{p}_{11} - 1}, \frac{\hat{p}_{00} - 1}{\hat{p}_{00} + \hat{p}_{11} - 1}\right] &= \frac{V(\hat{p}_{00})(-p_{11})}{(p_{00} + p_{11} - 1)^4} + \frac{V(\hat{p}_{11})(p_{00} - 1)}{(p_{00} + p_{11} - 1)^4} + O(n^{-2}).
\end{aligned}$$

Substituting these terms into Formula (29) and accounting for Formula (28) yields:

$$\begin{aligned}
V(\hat{\alpha}_p) &= \frac{V(\hat{p}_{00}) \left[E[\hat{\alpha}^*]^2 - 2p_{11}E[\hat{\alpha}^*] + p_{11}^2 \right]}{(p_{00} + p_{11} - 1)^4} \\
&\quad + \frac{V(\hat{p}_{11}) \left[E[\hat{\alpha}^*]^2 - 2(1 - p_{00})E[\hat{\alpha}^*] + (1 - p_{00})^2 \right]}{(p_{00} + p_{11} - 1)^4} + O\left(\max\left[\frac{1}{n^2}, \frac{1}{N}\right]\right) \\
&= \frac{V(\hat{p}_{00}) [E[\hat{\alpha}^*] - p_{11}]^2}{(p_{00} + p_{11} - 1)^4} + \frac{V(\hat{p}_{11}) [E[\hat{\alpha}^*] - (1 - p_{00})]^2}{(p_{00} + p_{11} - 1)^4} + O\left(\max\left[\frac{1}{n^2}, \frac{1}{N}\right]\right) \\
&= \frac{V(\hat{p}_{00})(1 - \alpha)^2}{(p_{00} + p_{11} - 1)^2} + \frac{V(\hat{p}_{11})\alpha^2}{(p_{00} + p_{11} - 1)^2} + O\left(\max\left[\frac{1}{n^2}, \frac{1}{N}\right]\right).
\end{aligned}$$

Finally, inserting the expressions for $V(\hat{p}_{00})$ and $V(\hat{p}_{11})$ from Lemma 1 yields:

$$\begin{aligned}
V(\hat{\alpha}_p) &= \frac{\frac{p_{00}(1-p_{00})}{n(1-\alpha)} \left[1 + \frac{\alpha}{n(1-\alpha)} \right] (1 - \alpha)^2}{(p_{00} + p_{11} - 1)^2} + \frac{\frac{p_{11}(1-p_{11})}{n\alpha} \left[1 + \frac{1-\alpha}{n\alpha} \right] \alpha^2}{(p_{00} + p_{11} - 1)^2} \\
&\quad + O\left(\max\left[\frac{1}{n^2}, \frac{1}{N}\right]\right),
\end{aligned}$$

from which expression (14) follows. This concludes the proof of Theorem 2.

Calibration estimator

We will now prove the bias and variance approximations for the calibration estimator $\hat{\alpha}_c$ that was defined in Equation (15).

Proof (of Theorem 3). To compute the expected value of $\hat{\alpha}_c$, we first compute its expectation conditional on the 4-vector $\mathbf{N} = (N_{00}, N_{01}, N_{10}, N_{11})$:

$$\begin{aligned}
E(\hat{\alpha}_c \mid \mathbf{N}) &= E\left[\hat{\alpha}^* \frac{n_{11}}{n_{+1}} + (1 - \hat{\alpha}^*) \frac{n_{10}}{n_{+0}} \mid \mathbf{N}\right] \\
&= \hat{\alpha}^* E\left[\frac{n_{11}}{n_{+1}} \mid \mathbf{N}\right] + (1 - \hat{\alpha}^*) E\left[\frac{n_{10}}{n_{+0}} \mid \mathbf{N}\right] \\
&= \hat{\alpha}^* E\left[E\left(\frac{n_{11}}{n_{+1}} \mid \mathbf{N}, n_{+1}\right) \mid \mathbf{N}\right] \\
&\quad + (1 - \hat{\alpha}^*) E\left[E\left(\frac{n_{10}}{n_{+0}} \mid \mathbf{N}, n_{+0}\right) \mid \mathbf{N}\right] \\
&= \frac{N_{+1}}{N} E\left[\frac{1}{n_{+1}} n_{+1} \frac{N_{11}}{N_{+1}} \mid \mathbf{N}\right] + \frac{N_{+0}}{N} E\left[\frac{1}{n_{+0}} n_{+0} \frac{N_{10}}{N_{+0}} \mid \mathbf{N}\right] \\
&= \frac{N_{11}}{N} + \frac{N_{10}}{N} \\
&= \frac{N_{1+}}{N} = \alpha.
\end{aligned} \tag{30}$$

By the tower property of conditional expectations, it follows that $E[\hat{\alpha}_c] = E[E(\hat{\alpha}_c | \mathbf{N})] = \alpha$. This proves that $\hat{\alpha}_c$ is an unbiased estimator for α .

To compute the variance of $\hat{\alpha}_c$, we use the conditional variance decomposition, again conditioning on the 4-vector \mathbf{N} . We remark that N_{0+} and N_{1+} are deterministic values, but that N_{+0} and N_{+1} are random variables. As shown above in Equation (30), the conditional expectation is deterministic, hence it has no variance: $V(E[\hat{\alpha}_c | \mathbf{N}]) = 0$. The conditional variance decomposition then simplifies to the following:

$$V(\hat{\alpha}_c) = E[V(\hat{\alpha}_c | \mathbf{N})]. \quad (31)$$

The conditional variance $V(\hat{\alpha}_c | \mathbf{N})$ can be written as follows:

$$\begin{aligned} V[\hat{\alpha}_c | \mathbf{N}] &= V\left[\hat{\alpha}^* \frac{n_{11}}{n_{+1}} + (1 - \hat{\alpha}^*) \frac{n_{10}}{n_{+0}} \mid \mathbf{N}\right] \\ &= (\hat{\alpha}^*)^2 V\left[\frac{n_{11}}{n_{+1}} \mid \mathbf{N}\right] + (1 - \hat{\alpha}^*)^2 V\left[\frac{n_{10}}{n_{+0}} \mid \mathbf{N}\right] \\ &\quad + 2\hat{\alpha}^*(1 - \hat{\alpha}^*)C\left[\frac{n_{11}}{n_{+1}}, \frac{n_{10}}{n_{+0}} \mid \mathbf{N}\right]. \end{aligned} \quad (32)$$

We will consider these terms separately. First, the variance of n_{11}/n_{+1} can be computed by applying an additional conditional variance decomposition:

$$V\left[\frac{n_{11}}{n_{+1}} \mid \mathbf{N}\right] = V\left[E\left(\frac{n_{11}}{n_{+1}} \mid \mathbf{N}, n_{+1}\right) \mid \mathbf{N}\right] + E\left[V\left(\frac{n_{11}}{n_{+1}} \mid \mathbf{N}, n_{+1}\right) \mid \mathbf{N}\right].$$

The first term is zero, which can be shown as follows:

$$\begin{aligned} V\left[E\left(\frac{n_{11}}{n_{+1}} \mid \mathbf{N}, n_{+1}\right)\right] &= V\left[\frac{1}{n_{+1}} E(n_{11} \mid \mathbf{N}, n_{+1}) \mid \mathbf{N}\right] \\ &= V\left[\frac{1}{n_{+1}} n_{+1} \frac{N_{11}}{N_{+1}} \mid \mathbf{N}\right] \\ &= V\left[\frac{N_{11}}{N_{+1}} \mid \mathbf{N}\right] = 0. \end{aligned}$$

For the second term, we find under the assumption that $n \ll N$:

$$\begin{aligned} E\left[V\left(\frac{n_{11}}{n_{+1}} \mid \mathbf{N}, n_{+1}\right) \mid \mathbf{N}\right] &= E\left[\frac{1}{n_{+1}^2} V(n_{11} \mid \mathbf{N}, n_{+1}) \mid \mathbf{N}\right] \\ &= E\left[\frac{1}{n_{+1}^2} n_{+1} \frac{N_{11}}{N_{+1}} \left(1 - \frac{N_{11}}{N_{+1}}\right) \mid \mathbf{N}\right] \\ &= E\left[\frac{1}{n_{+1}} \mid \mathbf{N}\right] \frac{N_{11} N_{01}}{N_{+1}^2}. \end{aligned}$$

The expectation of $\frac{1}{n_{+1}}$ can be approximated with a second-order Taylor series:

$$\begin{aligned} V\left[\frac{n_{11}}{n_{+1}} \mid \mathbf{N}\right] &= \left[\frac{1}{E[n_{+1} \mid \mathbf{N}]} + \frac{1}{2} \frac{2}{E[n_{+1} \mid \mathbf{N}]^3} V[n_{+1} \mid \mathbf{N}]\right] \frac{N_{11}N_{01}}{N_{+1}^2} + O(n^{-3}) \\ &= \frac{1}{E[n_{+1} \mid \mathbf{N}]} \left[1 + \frac{V[n_{+1} \mid \mathbf{N}]}{E[n_{+1} \mid \mathbf{N}]^2}\right] \frac{N_{11}N_{01}}{N_{+1}^2} + O(n^{-3}) \\ &= \frac{1}{n\hat{\alpha}^*} \left[1 + \frac{1 - \hat{\alpha}^*}{n\hat{\alpha}^*}\right] \frac{N_{11}N_{01}}{N_{+1}^2} + O(n^{-3}). \end{aligned} \quad (33)$$

The variance of n_{10}/n_{+0} can be approximated in the same way, which yields the following expression:

$$V\left[\frac{n_{10}}{n_{+0}} \mid \mathbf{N}\right] = \frac{1}{n(1 - \hat{\alpha}^*)} \left[1 + \frac{\hat{\alpha}^*}{n(1 - \hat{\alpha}^*)}\right] \frac{N_{00}N_{10}}{N_{+0}^2} + O(n^{-3}). \quad (34)$$

Finally, it can be shown that the covariance in the final term is equal to zero:

$$\begin{aligned} C\left[\frac{n_{11}}{n_{+1}}, \frac{n_{10}}{n_{+0}} \mid \mathbf{N}\right] &= E\left[C\left(\frac{n_{11}}{n_{+1}}, \frac{n_{10}}{n_{+0}} \mid \mathbf{N}, n_{+0}, n_{+1}\right) \mid \mathbf{N}\right] \\ &\quad + C\left[E\left(\frac{n_{11}}{n_{+1}} \mid \mathbf{N}, n_{+0}, n_{+1}\right), E\left(\frac{n_{10}}{n_{+0}} \mid \mathbf{N}, n_{+0}, n_{+1}\right) \mid \mathbf{N}\right] \\ &= E\left[\frac{1}{n_{+0}n_{+1}} C(n_{11}, n_{10} \mid \mathbf{N}, n_{+0}, n_{+1}) \mid \mathbf{N}\right] \\ &\quad + C\left[\frac{1}{n_{+1}} E(n_{11} \mid \mathbf{N}, n_{+0}, n_{+1}), \frac{1}{n_{+0}} E(n_{10} \mid \mathbf{N}, n_{+0}, n_{+1}) \mid \mathbf{N}\right] \\ &= 0 + C\left[\frac{1}{n_{+1}} n_{+1} \frac{N_{11}}{N_{+1}}, \frac{1}{n_{+0}} n_{+0} \frac{N_{10}}{N_{+0}} \mid \mathbf{N}\right] = 0. \end{aligned} \quad (35)$$

Combining Formulas (33), (34) and (35) with (32) gives:

$$\begin{aligned} V[\hat{\alpha}_c \mid \mathbf{N}] &= \frac{N_{+1}^2}{N^2} \frac{1}{n\hat{\alpha}^*} \left[1 + \frac{1 - \hat{\alpha}^*}{n\hat{\alpha}^*}\right] \frac{N_{11}N_{01}}{N_{+1}^2} \\ &\quad + \frac{N_{+0}^2}{N^2} \frac{1}{n(1 - \hat{\alpha}^*)} \left[1 + \frac{\hat{\alpha}^*}{n(1 - \hat{\alpha}^*)}\right] \frac{N_{00}N_{10}}{N_{+0}^2} + O(n^{-3}) \\ &= \frac{1}{n\hat{\alpha}^*} \left[1 + \frac{1 - \hat{\alpha}^*}{n\hat{\alpha}^*}\right] \frac{N_{11}N_{01}}{N^2} \\ &\quad + \frac{1}{n(1 - \hat{\alpha}^*)} \left[1 + \frac{\hat{\alpha}^*}{n(1 - \hat{\alpha}^*)}\right] \frac{N_{00}N_{10}}{N^2} + O(n^{-3}). \end{aligned}$$

Recall from Formula (31) that $V[\hat{\alpha}_c] = E[V[\hat{\alpha}_c \mid \mathbf{N}]] = E[E[V[\hat{\alpha}_c \mid \mathbf{N}] \mid N_{+1}]]$. Hence,

$$\begin{aligned} V[\hat{\alpha}_c] &= E\left[\frac{1}{n\hat{\alpha}^*} \left(1 + \frac{1 - \hat{\alpha}^*}{n\hat{\alpha}^*}\right) E\left(\frac{N_{11}N_{01}}{N^2} \mid N_{+1}\right) \right. \\ &\quad \left. + \frac{1}{n(1 - \hat{\alpha}^*)} \left(1 + \frac{\hat{\alpha}^*}{n(1 - \hat{\alpha}^*)}\right) E\left(\frac{N_{00}N_{10}}{N^2} \mid N_{+1}\right)\right] + O(n^{-3}). \end{aligned} \quad (36)$$

To evaluate the expectations in this expression, we observe that, conditional on the column total N_{+1} , N_{11} is distributed as $\text{Bin}(N_{+1}, c_{11})$, where c_{11} is a calibration probability as defined in Section 2.5. Hence,

$$\begin{aligned} E[N_{11} | N_{+1}] &= N_{+1}c_{11} = \frac{N_{+1}\alpha p_{11}}{(1-\alpha)(1-p_{00}) + \alpha p_{11}} \\ V[N_{11} | N_{+1}] &= N_{+1}c_{11}(1-c_{11}). \end{aligned} \quad (37)$$

Similarly, since $N = N_{+1} + N_{+0}$ is fixed,

$$\begin{aligned} E[N_{00} | N_{+1}] &= N_{+0}c_{00} = \frac{N_{+0}(1-\alpha)p_{00}}{(1-\alpha)p_{00} + \alpha(1-p_{11})} \\ V[N_{00} | N_{+1}] &= N_{+0}c_{00}(1-c_{00}). \end{aligned} \quad (38)$$

Using these results, we obtain:

$$\begin{aligned} E\left[\frac{N_{11}N_{01}}{N^2} | N_{+1}\right] &= \frac{1}{N^2} E[N_{11}N_{01} | N_{+1}] \\ &= \frac{1}{N^2} E[N_{11}(N_{+1} - N_{11}) | N_{+1}] \\ &= \frac{1}{N^2} [N_{+1}E[N_{11} | N_{+1}] - E[N_{11}^2 | N_{+1}]] \\ &= \frac{1}{N^2} [N_{+1}E[N_{11} | N_{+1}] - V[N_{11} | N_{+1}] - E[N_{11} | N_{+1}]^2] \\ &= \frac{1}{N^2} [N_{+1}^2 c_{11} - N_{+1}c_{11}(1-c_{11}) - N_{+1}^2 c_{11}^2] \\ &= \frac{N_{+1}^2}{N^2} c_{11}(1-c_{11}) + O\left(\frac{1}{N}\right), \end{aligned} \quad (39)$$

and similarly

$$E\left[\frac{N_{00}N_{10}}{N^2} | N_{+1}\right] = \frac{N_{+0}^2}{N^2} c_{00}(1-c_{00}) + O\left(\frac{1}{N}\right). \quad (40)$$

Substituting expressions (39) and (40) into (36) and noting that $N_{+1}^2/N^2 = (\hat{\alpha}^*)^2$ and $N_{+0}^2/N^2 = (1-\hat{\alpha}^*)^2$, we obtain:

$$\begin{aligned} V[\hat{\alpha}_c] &= E\left[\frac{\hat{\alpha}^*}{n} \left(1 + \frac{1-\hat{\alpha}^*}{n\hat{\alpha}^*}\right) c_{11}(1-c_{11}) \right. \\ &\quad \left. + \frac{1-\hat{\alpha}^*}{n} \left(1 + \frac{\hat{\alpha}^*}{n(1-\hat{\alpha}^*)}\right) c_{00}(1-c_{00})\right] + O\left(\max\left[\frac{1}{n^3}, \frac{1}{Nn}\right]\right) \\ &= \left[\frac{E(\hat{\alpha}^*)}{n} + \frac{1-E(\hat{\alpha}^*)}{n^2}\right] c_{11}(1-c_{11}) \\ &\quad + \left[\frac{1-E(\hat{\alpha}^*)}{n} + \frac{E(\hat{\alpha}^*)}{n^2}\right] c_{00}(1-c_{00}) + O\left(\max\left[\frac{1}{n^3}, \frac{1}{Nn}\right]\right). \end{aligned}$$

Finally, substituting the expressions for $E(\hat{\alpha}^*)$ from (4) and the expressions for c_{11} and c_{00} from (37) and (38), the desired expression (17) is obtained. This concludes the proof of Theorem 3.

Comparing mean squared errors

To conclude, we present the proof of Theorem 4, which essentially shows that the mean squared error (up to and including terms of order $1/n$) of the calibration estimator is lower than that of the misclassification estimator.

Proof (of Theorem 4). Recall that the bias of $\hat{\alpha}_p$ as an estimator for α is given by

$$B[\hat{\alpha}_p] = \frac{p_{00} - p_{11}}{n(p_{00} + p_{11} - 1)} + O\left(\frac{1}{n^2}\right).$$

Hence, $(B[\hat{\alpha}_p])^2 = O(1/n^2)$ is not relevant for $\widetilde{MSE}[\hat{\alpha}_p]$. It follows that $\widetilde{MSE}[\hat{\alpha}_p]$ is equal to the variance of $\hat{\alpha}_p$ up to order $1/n$. From (14) we obtain:

$$\widetilde{MSE}[\hat{\alpha}_p] = \frac{1}{n} \left[\frac{(1 - \alpha)p_{00}(1 - p_{00}) + \alpha p_{11}(1 - p_{11})}{(p_{00} + p_{11} - 1)^2} \right]. \quad (41)$$

Recall that $\hat{\alpha}_c$ is an unbiased estimator for α , i.e., $B[\hat{\alpha}_c] = 0$. Also recall the notation $\beta = (1 - \alpha)(1 - p_{00}) + \alpha p_{11}$. It follows from (17) that the variance, and hence the MSE, of $\hat{\alpha}_c$ up to terms of order $1/n$ can be written as:

$$\begin{aligned} \widetilde{MSE}[\hat{\alpha}_c] &= \frac{1}{n} \left[\beta \frac{\alpha p_{11}}{\beta} \left(1 - \frac{\alpha p_{11}}{\beta} \right) + (1 - \beta) \frac{(1 - \alpha)p_{00}}{1 - \beta} \left(1 - \frac{(1 - \alpha)p_{00}}{1 - \beta} \right) \right] \\ &= \frac{\alpha(1 - \alpha)}{n} \left[\frac{(1 - p_{00})p_{11}}{\beta} + \frac{p_{00}(1 - p_{11})}{1 - \beta} \right]. \end{aligned} \quad (42)$$

To prove Expression (18), first note that

$$\frac{(1 - p_{00})p_{11}}{\beta} + \frac{p_{00}(1 - p_{11})}{1 - \beta} = \frac{(1 - p_{00})p_{11} + \beta(p_{00} - p_{11})}{\beta(1 - \beta)}. \quad (43)$$

The numerator of this equation can be rewritten as follows:

$$\begin{aligned} &(1 - p_{00})p_{11} + \beta(p_{00} - p_{11}) \\ &= (1 - p_{00})p_{11} + (1 - \alpha)p_{00}(1 - p_{00}) + \alpha p_{00}p_{11} - (1 - \alpha)(1 - p_{00})p_{11} - \alpha p_{11}^2 \\ &= (1 - \alpha)p_{00}(1 - p_{00}) + \alpha p_{00}p_{11} + \alpha(1 - p_{00})p_{11} - \alpha p_{11}^2 \\ &= (1 - \alpha)p_{00}(1 - p_{00}) + \alpha p_{11}(1 - p_{11}). \end{aligned}$$

Note that the obtained expression is equal to the numerator of Expression (41). Write $T = (1 - \alpha)p_{00}(1 - p_{00}) + \alpha p_{11}(1 - p_{11})$ for that expression. It follows that

$$\begin{aligned} &\widetilde{MSE}[\hat{\alpha}_p] - \widetilde{MSE}[\hat{\alpha}_c] \\ &= \frac{T}{n(p_{00} + p_{11} - 1)^2} - \frac{T\alpha(1 - \alpha)}{n\beta(1 - \beta)} \\ &= \frac{T}{n(p_{00} + p_{11} - 1)^2\beta(1 - \beta)} \left[\beta(1 - \beta) - \alpha(1 - \alpha)(p_{00} + p_{11} - 1)^2 \right]. \end{aligned}$$

Writing out the second factor in the last expression gives the following:

$$\begin{aligned}
& \beta(1 - \beta) - \alpha(1 - \alpha)(p_{00} + p_{11} - 1)^2 \\
&= (1 - \alpha)^2 p_{00}(1 - p_{00}) + \alpha(1 - \alpha) \left((1 - p_{00})(1 - p_{11}) + p_{00}p_{11} \right) + \alpha^2 p_{11}(1 - p_{11}) \\
&\quad - \alpha(1 - \alpha)(p_{00} + p_{11} - 1)^2 \\
&= (1 - \alpha)^2 p_{00}(1 - p_{00}) + \alpha(1 - \alpha) \left(p_{00}(1 - p_{00}) + p_{11}(1 - p_{11}) \right) + \alpha^2 p_{11}(1 - p_{11}) \\
&= (1 - \alpha)p_{00}(1 - p_{00}) + \alpha p_{11}(1 - p_{11}) \\
&= T.
\end{aligned}$$

This concludes the proof of Theorem 4.