Minimising quantifier variance under prior probability shift

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For the binary prevalence quantification problem under prior probability shift, we determine the asymptotic variance of the maximum likelihood estimator. We find that it is a function of the Brier score for the regression of the class label against the features under the test data set distribution. This observation suggests that optimising the accuracy of a base classifier on the training data set helps to reduce the variance of the related quantifier on the test data set. Therefore, we also point out training criteria for the base classifier that imply optimisation of both of the Brier scores on the training and the test data sets.

Keywords: Prior probability shift, quantifier, class distribution estimation, Cramér-Rao bound, maximum likelihood estimator, Brier score.

1 Introduction

The survey paper [7] described the problem to estimate prior class probabilities (also called prevalences) on a test set with a different distribution than the training set (the quantification problem) as “Given a labelled training set, induce a quantifier that takes an unlabelled test set as input and returns its best estimate of the class distribution.” As becomes clear from [7] and also more recent work on the problem, it has been widely investigated in the past twenty years.

A lot of different approaches to quantification of prior class probabilities has been proposed and analysed (see, e.g. [7, 8, 14]), but it appears that the following question has not yet received very much attention: Is it worth the effort to try to train a good (accurate) hard (or soft or probabilistic) classifier as the ‘base classifier’ for the task of quantification if the class labels of individual instances are unimportant and only the aggregate prior class probabilities are of interest?

Some researchers indeed suggest that the accuracy of the base classifiers is less important for quantification than for classification. [4] made the following statements:

• From the abstract of [4]: “These strengths can make quantification practical for business use, even where classification accuracy is poor.”

• P. 165 of [4]: “The effort to develop special purpose features or classifiers could increase the cost significantly, with no guarantee of an accurate classifier. Thus, an imperfect classifier is often all that is available.”

• P. 166 of [4]: “It is sufficient but not necessary to have a perfect classifier in order to estimate the class distribution well. If the number of false positives balances against false negatives, then the overall count of predicted positives is nonetheless correct. Intuitively, the estimation task is easier for not having to deliver accurate predictions on individual cases.”

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The point on the mutual cancellation of false positives and false negatives is mentioned also by a number of other researchers like for instance [3]. On p. 74, [3] wrote: “Equation 1 [with the definition of the $F_1$-measure] shows that $F_1$ deteriorates with $(FP + FN)$ and not with $|FP - FN|$, as would instead be required of a function that truly optimizes quantification.”

There are also researchers that hold the contrary position, at least as quantification under an assumption of prior probability shift (see 3.1 below for the formal definition) is concerned:

- [22] noted for the class of ‘ratio estimators’ they introduced that it was both desirable and feasible to construct estimators with small asymptotic variances.
- [19] demonstrated by a simulation study that estimating the prior class probabilities by means of a more accurate base classifier may entail much shorter confidence intervals for the estimates.
- [1] made a case for using the maximum likelihood estimator for the quantification task.

In the following, we revisit the question of the usefulness of accurate classifiers for quantification.

## 2 Related work

Prior probability shift is a special type of data set shift, see [13] for background information and a taxonomy of data set shift. In the literature, also other terms are used for prior probability shift, for instance ‘global drift’ [10] or ‘label shift’ [11].

The problem of estimating the test set prior class probabilities can also be interpreted as a problem to estimate the parameters of a ‘mixture model’ [5] where the component distributions are learnt on a training set. See [15] for an early work on the properties of the maximum likelihood (ML) estimator in this case. [17] revived the interest in the ML estimator for the unknown prior class probabilities in the test by specifying the associated ‘expectation maximisation’ (EM) algorithm.

The ML approach has been criticised for its sometimes moderate performance and the effort and amount of training data needed to implement it. However, recently some researchers [6, 1] began to vindicate the ML approach. [18] proposed to take recourse to the notion of Fisher consistency as a criterion to identify completely unsuitable approaches to the quantification problem. In contrast, he proved Fisher consistency of the ML estimator under prior probability shift.

In the following, we revisit the well-known asymptotic efficiency property of ML estimators in the special case of the ML estimator for prior class probabilities in the binary setting.

## 3 Setting

We consider the binary prevalence quantification problem in the following setting:

- There is a training (or source) data set $(x_1, y_1), \ldots, (x_m, y_m) \in \mathbb{X} \times \{0, 1\}$. It is assumed to be an i.i.d. sample of a random vector $(X, Y)$ with values in $\mathbb{X} \times \{0, 1\}$. The vector $(X, Y)$ is defined on a probability space $(\Omega, P)$, the training (or source) domain. The elements $\omega$ of $\Omega$ are the instances (or objects). Each instance $\omega$ belongs to one of the classes 0 and 1, and its class label is $Y(\omega) \in \{0, 1\}$. In addition, each instance $\omega$ has features $X(\omega) \in \mathbb{X}$. Often, $\mathbb{X}$ is the $d$-dimensional Euclidian space such that accordingly $X$ is a real-valued random vector. See Appendix B.1 of [24] for more detailed comments of how this setting avoids the logical problems that arise when feature vectors and instances are considered to be the same thing.

- Under the training distribution $P$, both the features $X(\omega)$ and the class labels $Y(\omega)$ of the instances are observed in a series of $m$ independent experiments resulting in the sample $(x_1, y_1), \ldots, (x_m, y_m)$. 
The sample can be used to infer the joint distribution of $X$ and $Y$ under $P$, and hence, in particular, also the distribution of $Y$ (the class distribution) under $P$.

- There is a test (or target) data set $z_1, \ldots, z_n \in \mathcal{X}$. It is assumed to be an i.i.d. sample of the random vector $X$ with values in $\mathcal{X}$, under a probability measure $Q$ on $\Omega$ that may be different to the training distribution $P$.

- Under the test distribution $Q$, only the features $X(\omega)$ of the instances are observed in a series of $n$ independent experiments resulting in the sample $z_1, \ldots, z_n$. The sample can be used to infer the distribution of $X$ under $Q$.

- The goal of quantification is to infer the distribution of $Y$ under $Q$, based on the sample of features $z_1, \ldots, z_n$ generated under $Q$ and on the joint sample of features and class labels $(x_1, y_1), \ldots, (x_m, y_m)$ generated under $P$. It is not possible to design a method for this inference without any assumption on the relation of $P$ and $Q$.

- In this paper, we assume that $P$ and $Q$ are related by prior probability shift, in the sense that the class-conditional feature distributions are the same under $P$ and $Q$, i.e. it holds that

$$P[X \in M | Y = i] = Q[X \in M | Y = i]$$

for $i \in \{0, 1\}$ and all measurable subsets $M$ of $\mathcal{X}$.

Denoting $P[Y = 1] = p$ and $Q[Y = 1] = q$, (3.1) implies that the distribution of the features $X$ under $P$ and $Q$ respectively can be represented as

$$P[X \in M] = p P[X \in M | Y = 1] + (1 - p) P[X \in M | Y = 0],$$

$$Q[X \in M] = q P[X \in M | Y = 1] + (1 - q) P[X \in M | Y = 0],$$

for $M \subset \mathcal{X}$. In the following, we assume that components $p, P[X \in M | Y = 1]$ and $P[X \in M | Y = 0]$ can be perfectly estimated from the training sample $(x_1, y_1), \ldots, (x_m, y_m)$.

Basically, this means letting $m = \infty$ which obviously is infeasible. It helps, however, to shed light on the importance of both maximum likelihood estimation and accurate classifiers for the efficient estimation of the unknown positive class prevalence $q$ in the test data set.

## 4 The ML estimator for the positive class prevalence

Assume that the conditional distributions in (3.1) have positive densities $f_i$, $i = 0, 1$. Then the unconditional density of the features vector $X$ under $Q$ is

$$f^Q(x) = (1 - q) f_0(x) + q f_1(x), \quad x \in \mathcal{X}.$$  

(4.1)

Hence the likelihood function $L(q) = L(q; z_1, \ldots, z_n)$ for the sample $z_1, \ldots, z_n$ is given by

$$L_n(q) = \prod_{i=1}^{n} \left( q (f_1(z_i) - f_0(z_i)) + f_0(z_i) \right).$$  

(4.2)

This implies for the first two derivatives of the log-likelihood with respect to $q$:

$$\frac{\partial \log L_n(q)}{\partial q} = \sum_{i=1}^{n} \frac{f_1(z_i) - f_0(z_i)}{q (f_1(z_i) - f_0(z_i)) + f_0(z_i)},$$  

(4.3a)

$$\frac{\partial^2 \log L_n(q)}{\partial q^2} = -\sum_{i=1}^{n} \left( \frac{f_1(z_i) - f_0(z_i)}{q (f_1(z_i) - f_0(z_i)) + f_0(z_i)} \right)^2 \leq 0.$$  

(4.3b)
We assume that there is at least one \( j \in \{1, \ldots, n\} \) such that
\[
 f_1(z_j) \neq f_0(z_j). \tag{4.4}
\]
Under (4.4), \( q \mapsto \log L_n(q) \) is strictly concave in \([0, 1]\). Hence (see Example 4.3.1 of [21]) the equation
\[
 \frac{\partial \log L_n(q)}{\partial q} = 0 \tag{4.5}
\]
has a solution \( 0 < q < 1 \) if and only if
\[
 \frac{1}{n} \sum_{i=1}^{n} \frac{f_1(z_i)}{f_0(z_i)} > 1 \quad \text{and} \quad \frac{1}{n} \sum_{i=1}^{n} \frac{f_0(z_i)}{f_1(z_i)} > 1. \tag{4.6a}
\]
This solution is then the unique point in \([0, 1]\) where \( L_n(q) \) takes its absolute maximum value. By strict concavity of \( \log L_n \), if (4.6a) is not true then either
\[
 \frac{1}{n} \sum_{i=1}^{n} \frac{f_1(z_i)}{f_0(z_i)} \leq 1 \quad \text{and} \quad \frac{1}{n} \sum_{i=1}^{n} \frac{f_0(z_i)}{f_1(z_i)} > 1, \tag{4.6b}
\]
applies or
\[
 \frac{1}{n} \sum_{i=1}^{n} \frac{f_1(z_i)}{f_0(z_i)} > 1 \quad \text{and} \quad \frac{1}{n} \sum_{i=1}^{n} \frac{f_0(z_i)}{f_1(z_i)} \leq 1, \tag{4.6c}
\]
holds. Under (4.6b), the unique maximum of \( \log L_n \) in \([0, 1]\) lies at \( q = 0 \) while under (4.6c), the unique maximum of \( \log L_n \) in \([0, 1]\) is taken at \( q = 1 \). In summary, under the natural assumption (4.4), the likelihood function \( L_n \) of (4.2) has an absolute maximum in \([0, 1]\) at a unique point \( \hat{q}_n \in [0, 1] \). As a consequence, the maximum likelihood (ML) estimate \( \hat{q}_n \) of the test set positive class prevalence \( q \) is well-defined as this \( \hat{q}_n \).

5 The Cramér-Rao bound for the ML estimator

If the ML estimator \( \hat{q}_n \) as introduced in Section [3] is interpreted as a function of an i.i.d. sample from the distribution of the feature vector under the test distribution \( Q \), then its variance is bounded from below by the inverse of the Fisher information of the sample (Cramér-Rao bound, see, e.g., Corollary 7.3.10 of [2]):
\[
 \text{var}[\hat{q}_n] \geq \frac{1}{n EQ \left[ \left( \frac{\partial \log f(z)}{\partial q} (X) \right)^2 \right]} = \frac{1}{n EQ \left[ \left( \frac{f_1(X) - f_0(X)}{f_0(X)} \right)^2 \right]}, \tag{5.1}
\]
where \( EQ \) denotes the expected value under the mixture probability measure \( Q \) of (5.2). Actually, since \( \hat{q}_n \) is the ML estimator of \( q \), (5.2) is not only a lower bound of \( \text{var}[\hat{q}_n] \) but also its asymptotic variance in the sense that \( \sqrt{n}(\hat{q}_n - q) \) converges in distribution toward \( \mathcal{N} \left( 0, EQ \left[ \left( \frac{f_1(X) - f_0(X)}{f_0(X)} \right)^2 \right]^{-1} \right) \), the normal distribution with mean 0 and variance \( EQ \left[ \left( \frac{f_1(X) - f_0(X)}{f_0(X)} \right)^2 \right]^{-1} \) (see, e.g., Theorem 10.1.12 of [2]).

Hence, if the densities of the class-conditional feature distributions are known, the ML estimator of \( q \) has asymptotically the smallest variance of all estimators of \( q \) on i.i.d. samples from the test distribution of the features. This is demonstrated in the two upper panels of Table 4 of [19] which shows on simulated data that confidence intervals for \( q \) — which are primarily driven by the standard deviations of the estimator — based on the ML estimator are the shortest if the training sample is infinite and the test sample is large.
6 The asymptotic variance of the ML estimator

Denote by $\eta_Q(x)$ the posterior positive class probability given $X = x$ under $Q$. Then it holds that

$$
\eta_Q(x) = \frac{q f_1(x)}{f_0(x)}.
$$

(6.1)

This implies the following representation of the asymptotic variance of the ML estimator $\hat{q}_n$:

$$
E_Q \left[ \left( \frac{f_1(X) - f_0(X)}{f_0(X)} \right)^2 \right]^{-1} = \frac{q^2 (1 - q)^2}{E_Q [\eta_Q(X) - q]^2]
= \frac{q^2 (1 - q)^2}{\text{var}_Q[\eta_Q(X)]}. 
$$

(6.2)

Recall the following decomposition of the optimal Brier Score $BS_Q(X)$ for the problem to predict the class variable $Y$ from the features $X$ (under the test distribution $Q$):

$$
BS_Q(X) = E_Q [(Y - \eta_Q(x))^2]
= \text{var}_Q[Y] - \text{var}_Q[\eta_Q(X)]
= q (1 - q) - \text{var}_Q[\eta_Q(X)].
$$

(6.3)

In (6.3), the optimal Brier Score $BS_Q(X)$ is also called refinement loss, while $\text{var}_Q[Y]$ and $\text{var}_Q[\eta_Q(X)]$ are known as uncertainty and resolution respectively.

Hence, by (6.2), the asymptotic variance of the ML estimator $\hat{q}_n$ is reduced if a feature vector $X$ with greater resolution is found (or if the Brier Score with respect to $X$ decreases). For instance, if a feature vector $X'$ is a function of the feature vector $X$, i.e. it holds that $X' = F(X)$ for some function $F : \mathbb{X} \rightarrow \mathbb{X}'$, then it follows that $BS_Q(X') \geq BS_Q(X)$. This in turn implies by (6.3) and (6.2) for the asymptotic variances of the ML estimators $\hat{q}_n(X')$ and $\hat{q}_n(X)$ that

$$
\text{var}_Q[\hat{q}_n(X')] \geq \text{var}_Q[\hat{q}_n(X)].
$$

(6.4)

Observe that $X' = F(X)$ also implies $BS_P(X') \geq BS_P(X)$, i.e. also under the training distribution $P$, the posterior positive class probability $\eta_P(X)$ based on $X$ is a better predictor of $Y$ than $\eta_P(X')$ which is based on $X'$. By the assumption underlying this paper, $BS_P(X')$ and $BS_P(X)$ are observable while $BS_Q(X')$ and $BS_Q(X)$ are not, because the class label $Y$ is not observed in the test data set.

Hence, does $BS_P(X') \geq BS_P(X)$ imply $BS_Q(X') \geq BS_Q(X)$ and therefore also (6.4), thus generalising the implication “$X' = F(X) \Rightarrow (6.4)$”?

This paper has no fully general answer to this question. Instead we can only point to alternative conditions on $X'$ and $X$ that imply both $BS_P(X') \geq BS_P(X)$ and $BS_Q(X') \geq BS_Q(X)$, but are weaker than $X' = F(X)$.

Brier curves: Recall the notion of Brier curve from [9] (with the slightly modified definition of [20]). If the Brier curve for $\eta_P(X')$ dominates the Brier curve for $\eta_P(X)$, then by item 6) of Proposition 5.2 and Proposition 4.1 of [20], it follows that $BS_P(X') \geq BS_P(X)$ and $BS_Q(X') \geq BS_Q(X)$ hold.

ROC analysis: Recall the notion of Receiver Operating Characteristic (ROC) as defined, for instance, in [16]. If the ROC for the density ratio associated with $X$ dominates the ROC for the density ratio associated with $X'$, then by Remark 5.4 and Proposition 4.1 of [20], it follows that $BS_P(X') \geq BS_P(X)$ and $BS_Q(X') \geq BS_Q(X)$ hold.
7 Conclusions

In this paper, we have revisited the binary quantification problem, i.e. the problem of estimating a binary prior class distribution when training and test distributions are different.

- Specifically, under the assumption of prior probability shift we have looked at the asymptotic variance of the maximum likelihood (ML) estimator.
- We have found that this asymptotic variance is closely related to the Brier score for the regression of the class label variable $Y$ against the features vector $X$ under the test set distribution.
- We have pointed sufficient conditions with associated training criteria for minimising both the Brier score on the training data set and the Brier score on the test data set.
- These findings suggest methods to reduce the variance of the ML estimator of the prior class probabilities on the test data set. Due to the statistical consistency of ML estimators, by reducing the variance of the estimator also its mean squared error is minimised.

Results of a simulation study in [19] and theoretical findings in [22, 23] suggest that improving the accuracy of the base classifiers used for quantification helps to reduce not only the variance of ML estimators but also of other estimators.

However, these findings must be qualified in so far as the observations made in this paper apply only to the case where both training data set and test data set are large. This is a severe restriction indeed as [4] pointed out the importance of quantification methods specifically in the case of small training data sets, for cost efficiency reasons.

Further research on developing efficient quantifiers for small or moderate training and test data sets therefore is highly desirable. A promising step in this direction has already been done by [12], with a proposal for the selection of the most suitable quantifiers for problems on data sets with widely varying sizes.

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