Does quantification without adjustments work?

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Classification is the task of predicting the class labels of objects based on the observation of their features. In contrast, quantification has been defined as the task of determining the prevalence of the positive class labels in a target dataset. The simplest approach to quantification is Classify & Count where a classifier is optimised for classification on a training set and applied to the target dataset for the prediction of positive class labels. The number of predicted positive labels is then used as an estimate of the positive class prevalence in the target dataset. Since the performance of Classify & Count for quantification is known to be inferior its results typically are subject to adjustments. However, some researchers recently have suggested that Classify & Count might actually work without adjustments if it is based on a classifier that was specifically trained for quantification. We discuss the theoretical foundation for this claim and explore its potential and limitations with a numerical example based on the binormal model with equal variances.

Keywords: Classification, quantification, confusion matrix method, Bayes error.

1 Introduction

The formal definition of quantification as a machine learning task is often credited to Forman (2008) who wrote: “The quantification task for machine learning: given a limited training set with class labels, induce a quantifier that takes an unlabeled test set as input and returns its best estimate of the number of cases in each class. In other words, the quantification task is to accurately estimate the test class distribution via machine learning, but without assuming a large training set that is sampled at random from the test distribution. The input to a quantifier is a batch of cases, whereas a traditional classifier takes a single case at a time and predicts its single class (or a distribution of classes reflecting its uncertainty about that one case).”

At least since the 1960s (Gart and Buck, 1966), researchers and practitioners were aware of the need to track changes of the prior probabilities (or prevalences) of classes between different datasets. In the machine learning community, the topic received renewed attention after Saerens et al. (2002) suggested a powerful alternative to the confusion matrix method they considered the standard approach at the time.

Fawcett and Flach (2005) marked another milestone in the discussion of how to deal with changed prevalences when they noticed that as a consequence of different causalities there are different dataset shift regimes that need to be tackled in different ways. Since then a number of papers has been published

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with proposals of how to categorise different types of dataset shift (Storkey, 2009; Moreno-Torres et al., 2012; Kull and Flach, 2014).

There are two types of dataset shift between training and target dataset that can be easily characterised. Under covariate shift, the assumption is that the posterior (i.e. conditional) class probabilities are the same on the training and the target datasets. However, the distribution of the covariates (or features) may change. This change should be taken into account already when a classifier is learnt (Shimodaira, 2000; Sugiyama et al., 2007; Bickel et al., 2009). The other easily characterised dataset shift type is prior probability shift where the feature distributions conditional on the classes remain the same when datasets are switched. Typically, in this case, adjustments to the posterior class probabilities or decision thresholds are recommended in the literature (Elkan, 2001; Forman, 2008; Xue and Weiss, 2009; Hopkins and King, 2010; Bella et al., 2010). Another approach is the direct estimation of the changed prior probabilities by minimising the distance of the feature distributions on the training and target datasets (Saerens et al., 2002; Forman, 2008; González-Castro et al., 2013; Hofer and Krempl, 2013; Du Plessis and Sugiyama, 2014; Kawakubo et al., 2016).

Other types of dataset shift are less easy to describe and to deal with. Tasche (2014) defined the invariant density ratio dataset shift which generalises the prior probability shift in such a way that only ratios of feature densities but not the densities themselves are unchanged. A recent paper by Hofer (2015) is outstanding by dealing with the dataset shift under very weak assumptions on the structure of the shift. Esuli et al. (2010) suggested that specially trained classifiers (called quantifiers) can be used for the so-called Classify & Count quantification (Forman, 2008) without a need of adjustments to the estimates. Classify & Count means that a classifier is optimised for classification on a training set and applied to the target dataset for the prediction of positive class labels. The number of predicted positive labels is then used as an estimate of the positive class prevalence in the target dataset. The practical implementation of this proposal for binary classification and quantification has been explored in papers by Milli et al. (2013), Barranquero et al. (2015) and Esuli and Sebastiani (2015). In all these three papers, emphasis is put on the need to have the quantifier properly calibrated on the training dataset, in the sense that the number of objects predicted to be positive should be equal to the true number of positive objects.

The experiments by Milli et al. (2013) suggest that after all Classify & Count with adjustments works better than pure Classify & Count. In contrast, Barranquero et al. (2015) and Esuli and Sebastiani (2015) report Classify & Count quantification performance of the specially trained quantifiers that is at least comparable to the performance of classifiers with adjustments. Esuli and Sebastiani (2015) are somewhat ambiguous with respect to clearly stating all of their optimisation criteria. This is different to Barranquero et al. (2015) whose authors clearly say that the calibration criterion must be supplemented by a condition enforcing good classification. This is an intuitive requirement because, in particular, the complementarity of the two criteria of calibration and classification seem to guarantee uniqueness of the optimal quantifier.

In this paper, we discuss the theoretical foundations and limitations of quantification without adjustments and illustrate the insights with the classical example of the binormal model with equal variances (van Trees, 1968). We focus on analysis of the Q-measure approach by Barranquero et al. (2015) because it has been well and intuitively documented. Our first finding is that quantification without adjustments in principle may work if proper calibration on the training dataset is ensured and the positive class prevalences on the training and target datasets are the same or nearly the same. However, a second finding is that the Q-measure approach has to be deployed with care because the quantifiers resulting from it may be miscalibrated.

This paper is organised as follows: In Section 2 and its subsections, the theory of binary classification is revisited such that the theoretically best quantifiers can be identified. Based on the results from this section, in Section 3 the experiment of Barranquero et al. (2015) is replicated and reviewed in a fully
controlled environment. Section 4 concludes the paper.

2 Classifying for quantification

In order to be able to appropriately assess the merits and limitations of the proposal by Barranquero et al. (2015) we adopt a precise mathematical formalism. Based on this formalism, we can characterise locally optimal binary classifiers which are somewhat in between optimal Bayes classifiers and optimal Neyman-Pearson classifiers (van Trees, 1968, Section 2.2). The concept of local optimality allows us to explore the full potential of the Barranquero et al. proposal such that it becomes clear what are its theoretical merits and limitations and where there are issues with the practical implementation.

2.1 Locally optimal binary classifiers

We discuss binary classification and the properties of classifiers in a probabilistic setting specified by a probability space as it was done by many authors before (see, e.g. van Trees, 1968). The probability space $(\Omega, \mathcal{A}, P)$ describes the experiment of choosing an object at random. The object has a class label and features. The features can be observed immediately while, depending on whether the probability space is interpreted as a training sample or target sample (sometimes also called test sample), the label is also observable at once or can be observed only with some delay. We interpret $\mathcal{A}$ as the $\sigma$-field (see, e.g. Billingsley, 1995, Section 2) of all admissible events, including events that cannot yet be observed. In addition, we have a $\sigma$-field $\mathcal{H}$ which is the family of the events that can be observed now. The event $A$ with $A \in \mathcal{A}$ but $A \notin \mathcal{H}$ reveals the object’s class label. If $A$ occurs the object has got class label 1. If $A^c = \Omega \setminus A$ occurs the object’s label is $-1$.

Assumption 2.1

- $(\Omega, \mathcal{A}, P)$ is a probability space. This space describes the experiment of selecting an object from a population at random and observing its features and (typically with some delay) class label.
- $A \in \mathcal{A}$ is a fixed event with $0 < P[A] < 1$. If $A$ is observed, the object’s class label is 1, otherwise if $A^c = \Omega \setminus A$ is observed, the object’s class label is $-1$.
- $\mathcal{H} \subset \mathcal{A}$ is a sub-$\sigma$-field of $\mathcal{A}$ such that $A \notin \mathcal{H}$. $\mathcal{H}$ is the $\sigma$-field of immediately observable events and, in particular, features.

In a binary classification problem setting, typically there are random variables $X : \Omega \rightarrow \mathbb{R}^d$ for some $d \in \mathbb{N}$ (explanatory variables or scores) and $Y : \Omega \rightarrow \{-1, 1\}$ (dependent or class variable) such that $\mathcal{H} = \sigma(X)$ and $Y^{-1}(\{1\}) = A$.

In the setting of Assumption 2.1, typically one wants to make a prediction of an object’s class label (i.e. about whether or not event $A$ has occurred) based on the observable information captured in the events $H \in \mathcal{H}$. Each of these events $H$ defines a binary classifier in the following sense:

- If $H$ occurs the object’s label is predicted as 1.
- If $H^c = \Omega \setminus H$ occurs the object’s label is predicted as $-1$.

This way binary classifiers are identified with elements of $\mathcal{H}$. We therefore do not introduce extra notation for classifiers. Note that the object’s class $A$ does not define a classifier because by assumption we have $A \notin \mathcal{H}$.

Define the expected misclassification cost $L_{a,b}(H)$ for $H \in \mathcal{H}$ and fixed $a,b \geq 0$ with $a + b > 0$ by

$$L_{a,b}(H) = a P[H^c \cap A] + b P[H \cap A^c]. \quad (2.1)$$
According to (2.1), there is no cost for misclassification if the label is correctly predicted (i.e. if the event \((A \cap H) \cup (A^c \cap H^c)\) occurs). If \(1\) is predicted for true label \(-1\) (event \(H \cap A^c\), false positive), the cost is \(b\). If \(-1\) is predicted for true label \(1\) (event \(H^c \cap A\), false negative), the cost is \(a\). The misclassification cost \(L_{a,b}(H)\) is the expected cost for the classifier represented by event \(H\).

From Section 2.2 of van Trees (1968) or Section 1.3 of Elkan (2001), we know the optimal choice \(H^*\) (Bayes classifier) of \(H\) for minimising \(L_{a,b}(H)\):

\[
H^* \overset{\text{def}}{=} \{ P[A | \mathcal{H}] > \frac{b}{a+b} \} = \{ \omega \in \Omega : P[A | \mathcal{H}](\omega) > \frac{b}{a+b} \} = \arg \min_{H \in \mathcal{H}} L_{a,b}(H),
\]

(2.2)

where \(P[A | \mathcal{H}]\) denotes the conditional probability (or posterior probability) of \(A\) given \(\mathcal{H}\) as defined in standard text books on probability theory (e.g. Billingsley, 1995, Section 33). The following proposition shows that in some sense all classifiers of the shape

\[
H_q \overset{\text{def}}{=} \{ P[A | \mathcal{H}] > q \}, \quad 0 < q < 1,
\]

(2.3)

are local minimisers of \(L_{a,b}(H)\).

**Proposition 2.2** Under Assumption 2.1, let \(a,b \geq 0\) with \(a+b > 0\) be fixed. Define \(L_{a,b}(H)\) and \(H_q\) by (2.1) and (2.3) respectively. Let \(p_q = P[H_q]\). Then the following two statements hold:

(i) \(q < \frac{b}{a+b} \Rightarrow H_q = \arg \min_{H \in \mathcal{H}, P[H] \geq p_q} L_{a,b}(H)\).

(ii) \(q > \frac{b}{a+b} \Rightarrow H_q = \arg \min_{H \in \mathcal{H}, P[H] \leq p_q} L_{a,b}(H)\).

**Proof.** Let \(H \in \mathcal{H}\) be given. With some algebra\(^1\), it can be shown that

\[
L_{a,b}(H) = a P[A] + (b - (a + b) q) P[H] + (a + b) E[(q - P[A | \mathcal{H}]) 1_{H \cap H^c}] \\
+ (a + b) E[(q - P[A | \mathcal{H}]) 1_{H \cap H^c}] \\
\geq a P[A] + (b - (a + b) q) P[H] + (a + b) E[(q - P[A | \mathcal{H}]) 1_{H \cap H^c}] \\
\geq a P[A] + (b - (a + b) q) P[H] + (a + b) E[(q - P[A | \mathcal{H}]) 1_{H_q}].
\]

(2.4)

In case \(q < \frac{b}{a+b}\) we have \(b - (a + b) q > 0\). Then it holds that \((b - (a + b) q) P[H] \geq (b - (a + b) q) p_q\) for \(P[H] \geq p_q\). By (2.4), this implies (i).

In case \(q > \frac{b}{a+b}\) we have \(b - (a + b) q < 0\). Then it holds that \((b - (a + b) q) P[H] \geq (b - (a + b) q) p_q\) for \(P[H] \leq p_q\). From this observation and (2.4), statement (ii) follows. \(\square\)

**Proposition 2.2** is about ‘locally’ optimal classifiers in the sense that only classifiers with identical probability of predicting 1 are compared. We state this observation more precisely in item (i) of the following remark:

**Remark 2.3**

(i) We have \(H^* = H \frac{p_q}{p_q} \) for \(H^*\) as defined in (2.2). Hence the case \(q = \frac{b}{a+b}\) is not treated in Proposition 2.2 because it is covered by (2.2). Nonetheless, it is worth noting that Proposition 2.2 and (2.2) together imply that for all \(a,b \geq 0\) with \(a + b > 0\) and \(0 < q < 1\) it holds that

\[
H_q = \arg \min_{H \in \mathcal{H}, P[H] = p_q} L_{a,b}(H).
\]

(ii) In the case \(a = 0, b = (1 - P[A])^{-1}\), Proposition 2.2 (i) implies for all \(0 < q < 1\) that

\[
H_q = \arg \min_{H \in \mathcal{H}, P[H] \geq p_q} \frac{P[H \cap A^c]}{P[A^c]} = \arg \min_{H \in \mathcal{H}, P[H] \geq p_q} P[H | A^c].
\]

\(P[H | A^c]\) is called false positive rate (FPR).

\(^{1}\)\(\mathbf{1}_S\) denotes the indicator function of the set \(S\), i.e. \(\mathbf{1}_S(s) = 1\) for \(s \in S\) and \(\mathbf{1}_S(s) = 0\) for \(s \notin S\).
(iii) In the case \( a = P[A]^{-1} \) and \( b = 0 \), Proposition 2.2 (ii) implies for all \( 0 < q < 1 \) that

\[
H_q = \arg \max_{H \in \mathcal{H}} \frac{P[H \cap A]}{P[A]} = \arg \max_{H \in \mathcal{H}, P[H] \leq p_q} P[H | A].
\]

\( P[H | A] \) is called true positive rate (TPR).

As mentioned above, Proposition 2.2 may be interpreted as a result in between the characterisation of optimal Bayes classifiers and the optimal classifier (test) from the Neyman-Pearson lemma. The following theorem gives a precise statement of this observation.

**Theorem 2.4** Let \((\Omega_0, \mathcal{M}, \mu)\) be a measure space. Assume that \( Q^- \) and \( Q^+ \) are probability measures on \((\Omega_0, \mathcal{M})\) which are absolutely continuous with respect to \( \mu \). Assume furthermore that the densities \( f^- \) and \( f^+ \) of \( Q^- \) and \( Q^+ \) respectively are positive. Define the likelihood ratio \( \lambda \) by \( \lambda = \frac{f^+}{f^-} > 0 \). If the distribution of \( \lambda \) is continuous under \( Q^- \) and \( Q^+ \), i.e. \( Q^-[\lambda = \ell] = 0 = Q^+[\lambda = \ell] \) for all \( \ell > 0 \), then there is a number \( \ell^* > 0 \) with \( Q^-[\lambda > \ell^*] = Q^+[\lambda \leq \ell^*] \) such that

\[
\min_{M \in \mathcal{M}} \max(Q^-[M], Q^+[M^c]) = Q^-[\lambda > \ell^*].
\]  

(2.5)

**Proof.** Define the probability space \((\Omega, A, P)\) by

- \( \Omega = \Omega_0 \times \{-1, 1\} \) with projections \( X(\omega, c) = \omega \) and \( Y(\omega, c) = c \) for \( (\omega, c) \in \Omega \),
- \( A = \mathcal{M} \otimes \mathcal{P}((-1, 1)) = \sigma(X, Y) \),
- \( P[Y = -1] = 1/2 = P[Y = 1] \) as well as \( P[X \in M | Y = -1] = Q^-[M] \) and \( P[X \in M | Y = 1] = Q^+[M] \) for \( M \in \mathcal{M} \).

Then Assumption 2.1 is satisfied if \( A \) is chosen as \( A = \{Y = 1\} \) and \( \mathcal{H} \) is chosen as \( \mathcal{H} = \sigma(X) = \mathcal{M} \times \{\emptyset, \{-1, 1\}\} \). By construction of \( P \), it follows that the probability of \( A = \{Y = 1\} \) conditional on \( \mathcal{H} \) is given by

\[
P[Y = 1 | \mathcal{H}] = \frac{f^+ \circ X}{f^+ \circ X + f^- \circ X}.
\]

This implies for any \( 0 < q < 1 \)

\[
P[P[Y = 1 | \mathcal{H}] > q] = \frac{Q^-[\lambda > \frac{q}{1-q}] + Q^+[\lambda > \frac{q}{1-q}]}{2}.
\]

(2.6)

Fix \( M \in \mathcal{M} \) and let \( H = \{X \in M\} \). The assumption on the continuity of the distribution of \( \lambda \) under \( Q^- \) and \( Q^+ \) implies that

\[
\min_{M \in \mathcal{M}} \max(Q^-[M], Q^+[M^c]) < 1.
\]

For this proof, we therefore may assume without loss of generality that \( \max(Q^-[M], Q^+[M^c]) < 1 \) and hence \( 0 < P[H] < 1 \). Again by the assumption on the continuity of the distribution of \( \lambda \) under \( Q^- \) and \( Q^+ \), then (2.6) implies that there is \( q = q(H) \) such that \( P[H] = P[P[Y = 1 | \mathcal{H}] > q] \). From Remark 2.3 (ii) and (iii) now it follows that

\[
\max(Q^-[M], Q^+[M^c]) = \max(P[H | Y = -1], P[H^c | Y = 1])
\]

\[
\geq \max(P[P[Y = 1 | \mathcal{H}] > q | Y = -1], P[P[Y = 1 | \mathcal{H}] > q] | Y = 1)
\]

\[
= \max(Q^-[\lambda > \frac{q}{1-q}], Q^+[\lambda \leq \frac{q}{1-q}]).
\]

Since this holds for all \( M \in \mathcal{M} \) with \( \max(Q^-[M], Q^+[M^c]) < 1 \), we can conclude that

\[
\min_{M \in \mathcal{M}} \max(Q^-[M], Q^+[M^c]) \geq \min_{\ell > 0} \max(Q^-[\lambda > \ell], Q^+[\lambda \leq \ell]).
\]
The intermediate value theorem implies that there is an \( \ell^* \) such that \( Q^-[\lambda > \ell^*] = Q^+|\lambda \leq \ell^* \). Since \( \ell \mapsto Q^-|\lambda > \ell \) is non-increasing and \( \ell \mapsto Q^+|\lambda \leq \ell \) is non-decreasing, it follows that

\[
\min_{\ell>0} \max(Q^-[\lambda > \ell], Q^+|\lambda \leq \ell) = Q^-[\lambda > \ell^*].
\] 

\[\square\]

**Remark 2.5** One interpretation of Theorem 2.4 is as providing sort of a Minimax test for the decision between two simple hypotheses. The test problem is to distinguish \( Q^- \) and \( Q^+ \). Tests are characterised by observable sets \( M \in \mathcal{M} \) where \( \omega \in M \) means 'accept \( Q^+ \)' and \( \omega \notin M \) means 'reject \( Q^+ \) in favour of \( Q^- \). However, in contrast to the setting of the Neyman-Pearson lemma, none of the two hypotheses is considered more important than the other. Therefore, as expressed on the left-hand side of (2.5), an optimal test is meant to minimise the probabilities of the type I and II errors at the same time.

(2.5) shows that in a 'continuous' setting there is an optimal test under criterion (2.5) which is based on the likelihood ratio \( \lambda \), i.e. the ratio of the densities of the tested probability measures. Hence the structure of the optimal test is the same as for the optimal Neyman-Pearson test, the cost-optimal Bayes test and the Minimax optimal Bayes test (see van Trees, 1968, Section 2.2).

### 2.2 Application to quantification under prior probability shift

In contrast to Esuli and Sebastiani (2015) and Milli et al. (2013), Barranquero et al. (2015) specify the dataset shift problem they are going to tackle with their proposal: It is prior probability shift. We modify Assumption 2.1 accordingly.

**Assumption 2.6** We extend the setting of Assumption 2.1 by assuming that there is a second probability measure \( P_1 \) on \((\Omega, A)\). \( P_1 \) evolves from \( P \) by prior probability shift, i.e. the probabilities of sets \( H \in \mathcal{H} \) conditional on \( A \) and the probabilities of sets \( H \in \mathcal{H} \) conditional on \( A^c \) are the same under \( P \) and \( P_1 \):

\[
P[H \mid A] = P_1[H \mid A] \quad \text{and} \quad P[H \mid A^c] = P_1[H \mid A^c], \quad \text{for all} \ H \in \mathcal{H}.
\]

Under Assumption 2.6, we can describe for any classifier \( H \in \mathcal{H} \) the probability \( P_1[H] \) as an affine function of \( w = P_1[A] \):

\[
P_1[H] = w \left( P[H \mid A] - P[H \mid A^c] \right) + P[H \mid A^c]. \tag{2.7}
\]

In practice, the true positive rate (TPR) \( P[H \mid A] \) and the false positive rate (FPR) \( P[H \mid A^c] \) can be estimated (possibly with large potential bias) from the training set (in our setting: \((\Omega, A, P)\)) and the probability \( P_1[H] \) of an object to be classified as positive (after prior probability shift) can be estimated from the target set (in our setting: \((\Omega, A, P_1)\)). Then (2.7) can be solved for \( w = P_1[A] \) to obtain an estimate of the new prior probability of the positive class:

\[
P_1[A] = \frac{P_1[H] - P[H \mid A^c]}{P[H \mid A] - P[H \mid A^c]}. \tag{2.8}
\]

This approach is called **confusion matrix method** (Saerens et al., 2002). It has also been described as **Adjusted Count** approach (Forman, 2008) and has been deployed by practitioners at least since the 1960s (Gart and Buck, 1966).

In theory, for any classifier \( H \), (2.8) provides the adjustment needed to obtain an accurate estimate of the probability of the positive class from a potentially quite inaccurate estimate by \( P_1[H] \). Experiments by some research teams, however, have cast doubt on the appropriateness of this approach. Both good (Xue and Weiss, 2009; Hopkins and King, 2010) and unsatisfactory performance (Saerens et al., 2002; Forman, 2008) of the confusion matrix method have been reported. Other papers report mixed findings (Bella et al., 2010; González-Castro et al., 2013; Hofer and Kreml, 2013; Du Plessis and Sugiyama, 2014).
As (2.8) is valid only under prior probability shift (Assumption 2.6), performance issues with the confusion matrix method should not be a surprise in circumstances when there is little evidence of prior probability shift against other types of dataset shift (see Moreno-Torres et al., 2012, for a taxonomy of dataset shift types). But most if not all of the above-mentioned reports on the performance of the confusion matrix method refer to controlled environments with prior probability shift. A number of reasons have been identified to potentially negatively impact the confusion matrix method performance. Among them are class imbalance in the training set (Forman, 2008) and issues with the accurate estimation of TPR and FPR on the training set (Esuli and Sebastiani, 2015).

Although many other approaches to prior probability estimation have been proposed (Hofer and Krempl, 2013; Du Plessis and Sugiyama, 2014; Hofer, 2015; Kawakubo et al., 2016), no gold standard has yet emerged because all approaches appear to suffer from numerical problems to some extent.

This observation has led some authors to suggest that so-called quantifiers (classifiers, specifically developed for quantification) might be a viable solution (Esuli et al., 2010; Milli et al., 2013; Barranquero et al., 2015; Esuli and Sebastiani, 2015). In the notation of this paper, both classifiers and quantifiers are characterised by observable events $H \in \mathcal{H}$ which are interpreted as ‘predict positive’. The difference between the concepts of ‘classifier’ and ‘quantifier’ is the intended use, as explained in the quotation from Forman (2008) in Section 1:

- Classifiers are deployed for predicting the class labels of single objects. Therefore, development of a classifier typically involves minimising the expected loss of decisions about single objects (see, for instance, the right-hand-side of (2.2)).
- Quantifiers are deployed for estimating the prevalence of a class in a sample or population. Barranquero et al. (2015) have argued that this different purpose should be reflected in a different objective function for the development of a quantifier. They suggest that with an appropriate objective function, no adjustment like (2.8) would be needed.
- In their paper, Barranquero et al. (2015) suggest maximising a Q-measure criterion (see (2.12a) below). Their experiments were conducted in a prior probability shift setting (see Assumption 2.6). Similarly, Milli et al. (2013) report experimental results from a prior probability shift setting.
- As a different approach, Esuli et al. (2010) suggest minimising the Kullback-Leibler distance between the observed class distribution and the predicted class distribution on the training set. Implicitly, as they work with Support Vector Machines (Esuli and Sebastiani, 2015), they also apply some classification optimisation criterion. Esuli and Sebastiani only use ‘natural’ datasets such that their datashift environment cannot be characterised as prior probability shift.

In the following, we focus on the analysis of the approach proposed by Barranquero et al. (2015) to deal with prior probability shift. Analysis of the approach followed by Esuli and Sebastiani (2015) is harder because Esuli and Sebastiani do not specify their dataset shift assumption and because the performance of their approach seems to depend on their choice of the classifier development methodology (as support vector machines). Analysis and potential criticism of Esuli and Sebastiani (2015), therefore, is not undertaken in this paper. The results of Milli et al. (2013) are less controversial than those of Barranquero et al. (2015) and Esuli and Sebastiani (2015) because Milli et al. report superior quantification performance for adjusted classifiers.

For a fixed, unadjusted classifier specified by a set $H \in \mathcal{H}$, the absolute prediction error $|P_1[A] - P_1[H]|$ of the prevalence of the positive class in the target dataset is the combination of a decreasing and an increasing straight line if it is represented as a function of the true positive class prior probability $w = P_1[A]$:

$$
\mathcal{E}_H(w) = \begin{cases} 
  w \left( P[H | A] - P[H | A^c] - 1 \right) + P[H | A^c], & \text{for } w \leq \frac{P[H | A^c]}{P[H | A] + 1 - P[H | A]}, \\
  w \left( 1 - P[H | A] + P[H | A^c] \right) - P[H | A^c], & \text{otherwise}, 
\end{cases}
$$

(2.9)
Figure 1: Illustration of prediction error function (2.9).

See Figure 1 for an illustration of the absolute prediction error concept. The rationale for the three different curves is explained in Section 3 below. For the moment, if we ignore the question of how to minimise the absolute prediction error, the figure tells us that every classifier is a perfect predictor of one positive class prevalence in the target dataset. Unfortunately, it is not very helpful to know this because it is perfection in the way a broken clock is perfectly right once a day. Hence it is worthwhile to try and find out more about minimising the error as we do in the following.

(2.9) immediately implies the following result on error bounds for the prediction of the positive class prevalence by a classifier:

**Proposition 2.7** Under Assumption 2.6, the following inequality holds for any $H \in \mathcal{H}$:

$$|P_1[A] - P_1[H]| \leq \max(P[H \mid A^c], P[H^c \mid A]).$$

(2.10)

Proposition 2.7 shows that a classifier’s prediction error with regard to the positive class prevalence is controlled by the classifier’s false positive rate (FPR) $P[H \mid A^c]$ and its false negative rate (FNR) $P[H^c \mid A]$. Theorem 2.4 (or Remark 2.3 (ii) and (iii)) makes it possible to identify the optimal (in this case the Minimax) classifier with regard to the prediction of the positive class prevalence:

**Corollary 2.8** Under Assumption 2.6, define the classifiers $H_q$, $0 < q < 1$ by (2.3). Assume in addition, that the distribution of $P[A \mid H]$ is continuous under both $P[A \mid A]$ and $P[A^c \mid A]$. Then there is a number
0 < q^* < 1 with \( P[H_q^* | A^c] = 1 - P[H_q^* | A] \) such that

\[
\min_{H \in \mathcal{H}} \max \{ P[H | A^c], P[H^c | A] \} = P[H_q^* | A^c].
\]

Corollary 2.8 is nice in telling us which classifier uniformly over all possible values of the positive class prevalence minimises the prediction error for the positive class prevalence on the target dataset. Note the similarity between this classifier and the classifier serving as the basis for the ‘method X’ of Forman (2008). It is also interesting to see that ‘Method Max’ of Forman (2008) (maximise TPR - FPR) is a special case of (2.2) with \( a = 1/P[A], \ b = 1/(1 - P[A]) \).

But from (2.9) it follows that the prediction error \( \mathcal{E}_{H_q^*}(w) \) of \( H_q^* \) is zero if and only if \( w = 1/2 \), i.e. if the prior positive class probability on the target dataset is 50%. This may seem unsatisfactory in particular if the positive class prevalence \( P[A] \) on the training set is very different from 1/2. It might be more appropriate to have prediction error zero for \( w = P[A] \), i.e. if the positive class prevalence on the target dataset is the same as on the training set. For this case the following result applies:

**Corollary 2.9** Under Assumption 2.6, define the classifiers \( H_q, 0 < q < 1 \) by (2.3). Assume in addition, that there is a number \( 0 < r < 1 \) such that \( P[H_r] = P[A] \). Then it holds that

\[
\min_{H \in \mathcal{H}, P[H] = P[A]} \max \{ P[H | A^c], P[H^c | A] \} = \max \{ P[H_r | A^c], P[H_r^c | A] \}.
\]

It can be easily checked that for \( H_r \) from Corollary 2.9 we have \( \mathcal{E}_{H_r}(P[A]) = 0 \), with \( \mathcal{E} \) defined as in (2.9).

### 2.3 The Q-measure approach

Barranquero et al. (2015) define the **Normalized Absolute Score (NAS)** for measuring how well a classifier (characterised by a set \( H \in \mathcal{H} \), as explained below Assumption 2.1) predicts the prior class probabilities \( P[A] \) and \( 1 - P[A] \) in the binary classification setting as described by Assumption 2.1:

\[
\text{NAS}(H) \overset{\text{def}}{=} 1 - \frac{|P[H] - P[A]|}{\max(P[A], 1 - P[A])}.
\]  

(2.11a)

By definition, we have \( \text{NAS}(H) = 1 \) if and only if \( P[H] = P[A] \). Otherwise, the range of \( \text{NAS}(H) \) depends on the value of \( P[A] \). If \( P[A] \leq 1 - P[A] \), then \( P[H] = 0 \) implies \( \text{NAS}(H) = \frac{1 - 2P[A]}{1 - P[A]} \) and \( P[H] = 1 \) implies \( \text{NAS}(H) = 0 \). If \( P[A] > 1 - P[A] \), then \( P[H] = 0 \) implies \( \text{NAS}(H) = 0 \) and and \( P[H] = 1 \) implies \( \text{NAS}(H) = \frac{2P[A] - 1}{P[A]} \).

The dependence of the range of \( \text{NAS} \) on the value of \( P[A] \) is unsatisfactory because it makes comparison of \( \text{NAS} \) values computed for different underlying values of \( P[A] \) incommensurable and, potentially, could entail bias if \( \text{NAS} \) is used as an optimization criterion. The following alternative definition of \( \text{NAS}^* \) avoids these issues:

\[
\text{NAS}^*(H) \overset{\text{def}}{=} 1 - \frac{\max(P[H] - P[A], 0)}{P[A]} - \frac{\max(P[A] - P[H], 0)}{P[A]}.
\]  

(2.11b)

By this definition, we have \( \text{NAS}^*(H) = 1 \) if and only if \( P[H] = P[A] \), \( \text{NAS}^*(H) = 0 \) if and only if \( P[H] \in \{0, 1\} \), and \( 0 < \text{NAS}^*(H) < 1 \) otherwise. In the following, we use \( \text{NAS}^* \) instead of \( \text{NAS} \) in order to make sure that the full potential of the approach by Barranquero et al. (2015) is realised.

Barranquero et al. (2015) suggest training **reliable** classifiers in order to predict prior (unconditional) class probabilities on the target dataset under **prior probability shift**. With ‘reliability’ they mean that the classifiers in question should perform well in terms of being good at classification and being good at quantification at the same time.
In order to train an optimal quantifier for predicting the class probability $P[A]$, Barranquero et al. (2015) suggest to maximise for some $\beta > 0$ the $Q_\beta$-measure over all possible classifiers (characterised by the sets $H \in \mathcal{H}$ whose outcomes trigger the prediction of class 1):

\[
Q_\beta(H) \overset{\text{def}}{=} \frac{(1 + \beta^2) P[H | A] \text{NAS}(H)}{\beta^2 P[H | A] + \text{NAS}(H)}
\]

\[
= \frac{1 + \frac{\beta^2}{\text{NAS}(H) + P[H | A]}}{P[H | A]}
\]

By the definitions of $P[H | A]$ and NAS($H$) the denominator on the right-hand side of (2.12a) takes the value 0 if and only if $P[H] = 0$. Representation (2.12b) of $Q_\beta(H)$ implies $\lim_{P[H] \to 0} Q_\beta(H) = 0$. Therefore we can define $Q_\beta(H)$ by (2.12a) for $H \in \mathcal{H}$ with $P[H] > 0$ and $Q_\beta(H) = 0$ for $H \in \mathcal{H}$ with $P[H] = 0$.

$Q_\beta(H)$ is a weighted harmonic mean of the true positive rate $P[H | A]$ and the normalized absolute score and, as such, is increasing in both $P[H | A]$ and NAS($H$). Barranquero et al. (2015) suggest that by maximising $Q_\beta(H)$ over $H$ for fixed $A$ on a training set, the resulting classifier should be able to provide good estimates of $P_1[A]$ on target datasets with possibly different prior class distributions.

Using the observation from Remark 2.3 (iii), in Section 3 we demonstrate by the standard example of a binormal model that optimal classifiers with respect to $Q_\beta$ in general are not best quantifiers. First note that Remark 2.3 (iii) implies the following result.
**Proposition 2.10** Under Assumption 2.1, define $Q_β(H)$, $H ∈ ℋ$ by (2.12a) and $H_q$, $q ∈ (0, 1)$ by (2.3). For $0 < u < 1$ denote by $q(u)$ the $u$-quantile\(^2\) of $P[A|ℋ]$. If the distribution of $P[A|ℋ]$ is continuous then it holds that
\[
\sup_{H ∈ ℋ} Q_β(H) = \sup_{P[A] ≤ u < 1} Q_β(H_{q(1−u)}).
\] (2.13)

**Proof.** Observe that $\sup_{H ∈ ℋ} Q_β(H) = \sup_{H ∈ ℋ, 0 < P[H] < 1} Q_β(H)$ since $Q_β(H) = 0$ for $P[H] = 0$ and $P[H] = 1$.

Fix $H ∈ ℋ$ with $0 < P[H] < 1$. By continuity of $x ↦ P[P[A|ℋ] ≤ x]$, then we have $P[H_{q(u)}] = P[H]$ for $u = 1 − P[H]$. Hence Remark 2.3 (iii) implies
\[
Q_β(H) = \frac{1 + β^2}{\text{NAS}(H_{q(u)}) + \frac{1}{P[H|ℋ]}} \leq \frac{1 + β^2}{\text{NAS}(H_{q(u)}) + \frac{1}{Q[H_{q(u)}]|ℋ}} = Q_β(H_{q(u)}).
\]

This implies
\[
\sup_{H ∈ ℋ} Q_β(H) = \sup_{0 < u < 1} Q_β(H_{q(1−u)}).
\]

However, for $0 < u ≤ P[A]$ both $P[H_{q(1−u)}|A]$ and $\text{NAS}(H_{q(1−u)})$ are non-decreasing in $u$. Hence it follows that $Q_β(H_{q(1−u)}) ≤ Q_β(H_{q(1−P[A])})$ for $0 < u ≤ P[A]$ and therefore (2.13).

See Figure 2 for an illustration of Proposition 2.10. Unfortunately, in practice most of the time it is not possible to accurately estimate general posterior probabilities like $P[A|ℋ]$. This has led some authors to propose workarounds like the one by Platt (2000) which do not necessarily deliver good results. However, the following corollary describes a special setting in which the right-hand side of (2.13) can be considerably simplified.

**Corollary 2.11** Under Assumption 2.1, define $Q_β(H)$, $H ∈ ℋ$ by (2.12a) and $H_q$, $q ∈ ℝ$ by (2.3). Make these two additional assumptions:

(i) There is a real random variable $X$ on $(Ω, ℛ, P)$ with continuous distribution such that $ℋ ⊇ σ(X)$, i.e. $X$ is $ℋ$-measurable.

(ii) There is a continuous function $f : ℝ → [0, 1]$ such that $P[A|ℋ] = f(X)$.

The function $f$ is either strictly increasing with $\lim_{x → −∞} f(x) = 0$ and $\lim_{x → ∞} f(x) = 1$ or strictly decreasing with $\lim_{x → −∞} f(x) = 1$ and $\lim_{x → ∞} f(x) = 0$.

Then if $f$ is increasing it holds that
\[
\sup_{H ∈ ℋ} Q_β(H) = \sup_{P[A] ≤ u ≤ 1} Q_β(\{X > q_1−u(X)\}).
\]

Otherwise, if $f$ is decreasing it holds that
\[
\sup_{H ∈ ℋ} Q_β(H) = \sup_{P[A] ≤ u ≤ 1} Q_β(\{X < q_u(X)\}).
\]

**Proof.** Follows from Proposition 2.10 because $H_{q(1−u)} = \{X > q_1−u(X)\}$ in the case of increasing $f$ and $H_{q(1−u)} = \{X < q_u(X)\}$ in the case of decreasing $f$, for $P[A] ≤ u < 1$.

Corollary 2.11 allows us in Section 3 to replicate the experiment by Barranquero et al. (2015) in a fully controlled environment such that the merits and limitations of their approach can carefully be studied.

\(^2\)For a real random variable $X$ and $α ∈ (0, 1)$, the $α$-quantile $q_α(X)$ of $X$ is defined by $q_α(X) = \inf\{x ∈ ℝ : P[X ≤ x] ≥ α\}$. 

11
3 The binormal case with equal variances

We consider the binormal model with equal variances as an example that fits into the setting of Assumption 2.1 and Corollary 2.11.

- $\Omega = \mathbb{R} \times \{-1, 1\}$, $\mathcal{A} = \mathcal{B}(\mathbb{R}) \otimes \mathcal{P}(\{-1, 1\})$ where $\mathcal{B}(\mathbb{R})$ denotes the Borel-$\sigma$-field on $\mathbb{R}$ and $\mathcal{P}(\{-1, 1\})$ is the power set of $\{-1, 1\}$.
- On $\Omega$, we define the projections $X$ and $Y$, i.e. for $\omega = (x, y) \in \Omega$ we let $X(\omega) = x$ and $Y(\omega) = y$.
- $A = \{Y = 1\} \not\in \mathcal{H} = \sigma(X)$.
- $P$ is defined by specifying the marginal distribution of $Y$ with $P[A] = p \in (0, 1)$, and defining the conditional distribution of $Y$ given $X$ as normal distributions with equal variances:

$$P[X \in \cdot | A] = \mathcal{N}(\nu, \sigma^2),$$
$$P[X \in \cdot | A^c] = \mathcal{N}(\mu, \sigma^2).$$

(3.1a)

In (3.1a), we assume that $\mu < \nu$ and $\sigma > 0$. (3.1a) implies that the distribution of $X$ is given by a mixture of normal distributions$^3$

$$P[X \leq x] = p \Phi \left( \frac{x - \nu}{\sigma} \right) + (1 - p) \Phi \left( \frac{x - \mu}{\sigma} \right), \quad x \in \mathbb{R}. \quad (3.1b)$$

- The posterior probability $P[A|\mathcal{H}]$ in this setting is given by

$$P[A|\mathcal{H}] = \frac{1}{1 + \exp(aX + b)}, \quad (3.2)$$

with $a = \frac{\mu - \nu}{\sigma^2} < 0$ and $b = \frac{\nu^2 - \mu^2}{2\sigma^2} + \log \left( \frac{1-p}{p} \right)$.

We replicate the experiment of Barranquero et al. (2015) in this setting:

- We look at a training set $(\Omega, \mathcal{A}, P)$ and a target dataset $(\Omega, \mathcal{A}, P_1)$. The probability measures $P$ and $P_1$ are defined as $P$ above but with (possibly) different values of $P[A] = p$ and $P_1[A] = p_1$, respectively.
- We “train” a classifier on the training set $(\Omega, \mathcal{A}, P)$ by maximising $Q_\beta$ as given by (2.12a). Classifiers can be identified with sets $H \in \mathcal{H}$ in the sense that the prediction is the positive class $A$ if $H$ occurs and the negative class $A^c$ otherwise. “Training” in the binormal setting actually means to make use of Corollary 2.11 in order to identify the optimal classifier $H^*$. The following formulae are used for the optimization of $Q_\beta$:

$$P[X > q_{1-u}(X) | A] = 1 - \Phi \left( \frac{q_{1-u}(X) - \nu}{\sigma} \right), \quad (3.3a)$$
$$\text{NAS}^*(\{X > q_{1-u}(X)\}) = 1 - \max \left( \frac{u - p}{1-p}, \frac{0}{p} \right) = \frac{\max(p - u, 0)}{p}. \quad (3.3b)$$

The quantile $q_{1-u}(X)$ (see footnote 2 for its definition) must be numerically determined by solving for $x$ the following equation:

$$1 - u = p_0 \Phi \left( \frac{x - \nu}{\sigma} \right) + (1 - p_0) \Phi \left( \frac{x - \mu}{\sigma} \right). \quad (3.4)$$

As the optimization problem has no closed-form solution, we apply the R-function 'optimize' (R Development Core Team, 2010) to find the optimal classifier $H^* = \{X > q_{1-u^*}(X)\}$. $^3\Phi$ denotes the standard normal distribution function $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-y^2/2} dy.$
We evaluate the $Q_\beta$-optimal classifier $H^*$ on the target dataset $(\Omega, A, P_1)$ by calculating $P_1[H^*]$ and compare its value to $p_1 = P_1[A]$ in order to check how good the Classify & Count approach (Forman, 2008) based on $H^*$ is. We compare the performance of $H^*$ with two other classifiers: the Minimax classifier $H_{\text{Mini}}$ from Corollary 2.8 and the locally best classifier $H_{\text{loc}}$ from Corollary 2.9.

This means that we need to evaluate (2.9) for the three classifiers. For this purpose, the following formulae are used:

\begin{align}
P[H^* | A] &= \Phi \left( \frac{q_{1-u^*}(X) - \nu}{\sigma} \right), \quad P[H^* | A^c] = \Phi \left( \frac{q_{1-u^*}(X) - \mu}{\sigma} \right); \quad (3.5a) \\
P[H_{\text{Mini}} | A] &= \Phi \left( \frac{\nu^*}{2} - \frac{\nu}{\sigma} \right), \quad P[H_{\text{Mini}} | A^c] = \Phi \left( \frac{\mu^*}{2} - \frac{\mu}{\sigma} \right); \quad (3.5b) \\
P[H_{\text{loc}} | A] &= \Phi \left( \frac{q_{1-p}(X) - \nu}{\sigma} \right), \quad P[H_{\text{loc}} | A^c] = \Phi \left( \frac{q_{1-p}(X) - \mu}{\sigma} \right). \quad (3.5c)
\end{align}

For the calculations, we have used the following parameters:

\[ \mu = 0, \quad \nu = 2, \quad \sigma = 1, \quad P[A] = p = 25\%. \quad (3.6) \]

The results of the calculations are shown in Figures 2 and 1. Figure 2 presents graphs of $u \mapsto Q_\beta(\{X > q_{1-u}(X)\})$ in the binormal setting of this section, with parameters chosen as in (3.6). The Q-measure $Q_\beta$ is defined by (2.12b), but we use $\text{NAS}^*$ instead of $\text{NAS}$. The solid curve is for $\beta = 1$, where equal weights are put on $\text{NAS}^*$ and the TPR $P[H | A]$, and the dashed curve is for $\beta = 2$, where the weight put on $\text{NAS}^*$ is four times the weight for the TPR.

The kinks in both graphs of Figure 2 are due to the fact that

\[ u \mapsto \text{NAS}^*(\{X > q_{1-u}(X)\}) = 1 - \frac{\max(u-p,0)}{1-p} - \frac{\max(p-u,0)}{p}, \quad 0 \leq u \leq 1, \]

is not differentiable in $u = p$. The function $u \mapsto \text{NAS}$ would not be differentiable in $u = p$ either. Both curves have a unique maximum which is at $u = p = 0.25$ for $\beta = 2$ and at some $u > p = 0.25$ for $\beta = 1$.

Hence the graph for $\beta = 2$ has its maximum at that $u$ where $\text{NAS}^*(\{X > q_{1-u}(X)\})$ takes its maximum value 1. As a consequence, in the case $\beta = 2$, the $Q_\beta$-optimal classifier is identical with the locally best classifier according to Corollary 2.9.

In contrast, in the case $\beta = 1$, for $u$ slightly greater than $p = 0.25$ the decline in value of $\text{NAS}^*(\{X > q_{1-u}(X)\})$ is over-compensated by a rise in the value of the TPR such that the maximum is incurred at some $u > p$. The consequence of this for the error (2.9) in the prediction of a target dataset positive class prevalence is displayed in Figure 1.

Figure 1 shows that by incident the error-performance of the $Q_\beta$-optimal classifier for $\beta = 1$ is close to the performance of the Minimax classifier identified in Corollary 2.8. Nonetheless, its performance would be deemed unsatisfactory if the true positive class prevalence in the target dataset were the same or nearly the same as the assumed positive class prevalence of 25% in the training dataset. In that case, clearly the locally best classifier as identified by the $Q_\beta$-measure for $\beta = 2$ or by Corollary 2.9 would perform much better and even perfectly if the training and target prevalences were the same.

### 4 Conclusions

We have investigated a claim by Barranquero et al. (2015) and Esuli and Sebastiani (2015) that binary class prevalences on target datasets can be estimated by classifiers without further adjustments if these
classifiers are developed as so-called quantifiers on the training datasets. The development of such quantifiers involves special optimisation criteria covering both calibration (i.e. the number of objects predicted as positive equals the true number of positives) and classification power.

Barranquero et al. (2015) recommended the so-called Q-measure as the optimisation criterion for the quantifier and tested their approach on some real-world datasets. It is not fully clear, however, from Barranquero et al. (2015) which of their observations are fundamental and which are sample-driven and incidental. In this paper, therefore, we have identified the theoretically correct way to determine the best quantifiers according to the Q-measure criterion. We then have replicated the experiment of Barranquero et al. (2015) in the fully controlled setting of the binormal model with equal variances. For binary classification settings, we have found that

1) quantification without adjustments in principle may work if proper calibration on the training dataset is ensured and the positive class prevalences on the training and target datasets are the same or nearly the same, and

2) the Q-measure approach has to be deployed with care because the quantifiers resulting from it may be miscalibrated.

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