Calibrating sufficiently

Dirk Tasche*

When probabilistic classifiers are trained and calibrated, the so-called grouping loss component of the calibration loss can easily be overlooked. Grouping loss refers to the gap between observable information and information actually exploited in the calibration exercise. We investigate the relation between grouping loss and the concept of sufficiency, identifying comonotonicity as a useful criterion for sufficiency. We revisit the probing reduction approach of Langford and Zadrozny (2005) and find that it produces an estimator of probabilistic classifiers that reduces grouping loss. Finally, we discuss Brier curves as tools to support training and ‘sufficient’ calibration of probabilistic classifiers.

Keywords: Probabilistic classifier, calibration, Brier score, sufficiency, probing reduction, Brier curve.

2020 Mathematics Subject Classification: 62B05, 62P99

1. Introduction

Binary classification, in the first place, deals with decision tools (classifiers) that facilitate the prediction of the classes of instances on the basis of the so-called features of the instances. Accordingly, the simplest classifiers are crisp (or discrete) in the sense of having the set \{0, 1\} as output range: 1 for ‘predict positive class’, 0 for ‘predict negative class’. Scoring (or soft) classifiers provide output in a continuous range, usually with the interpretation that high values indicate high likelihood of the instance belonging to the positive class, while low values suggest that membership of the negative class is more likely.

In many applications of classification, there is a need for ‘calibrated’ probabilistic classifiers which reflect the likelihood of the positive class given the features of an instance in a frequentist statistical sense (Platt, 2000; Zadrozny and Elkan, 2002; Cohen and Goldszmidt, 2004; Kull et al., 2017). How to best achieve good calibration and how to measure it are active research areas (Böken, 2021; Roelofs et al., 2020).

In this paper, we argue that for attaining good calibration of a probabilistic classifier the so-called ‘grouping loss’ (Kull and Flach, 2014) must not be neglected. We show that grouping loss reflects an information gap that is caused by not fully exploiting the information provided by the features when learning the probabilistic classifier.

Most of the bits and pieces needed for a thorough discussion of grouping loss are available in the literature:

- Sufficiency and admissibility (see Devroye et al. (1996), Section 32.3)
- Probing reduction (Langford and Zadrozny, 2005)
- Brier curves (Hernández-Orallo et al., 2011)

In this paper, we put these pieces together and explain how they complement each other. The paper, in particular, presents the following new contributions to the subject:

- We point out that the common practice of first developing a so-called scoring classifier and then calibrating it to obtain a probabilistic classifier risks loss of accuracy (as measured by the Brier

*Swiss Financial Market Supervisory Authority (FINMA). The opinions expressed in this note are those of the author and do not necessarily reflect views of FINMA.

Email: dirk.tasche@gmx.net
score) unless the scoring classifier is strongly comonotonic with the posterior probability of the positive class (Proposition 3.7).

- We extend the findings on sufficiency by Bröcker (2009) (Proposition 3.10) and present a counter-example to the ‘if’-part of Theorem 10.2 of Schervish (1989) (Example 3.12).
- We provide a more general representation of the ‘probing predictor’ of Langford and Zadrozny (2005) as well as a rigorous proof of their Theorem 2 (Theorem 4.2 below).
- We determine, in full generality, the point where the Brier curve of a calibrated probabilistic classifier takes its maximum (Proposition 5.2) and derive a novel lower bound for the Brier score associated with a binary regression problem (Proposition 5.5).
- Following Holzmann and Eulert (2014), we argue that the concept of $\sigma$-fields from measure theory is best-suited for analysing the role of information in the calibration of probabilistic classifiers.

We set the stage for the paper in Section 2 where we also state more formally the problem. In Sections 3, 4 and 5 respectively, then the concept of sufficiency, probing reduction, and Brier curves are discussed in detail. Section 5.3 provides a recommendation of how to avoid or at least control grouping loss, or in other words how to achieve ‘sufficient calibration’. The paper concludes with a summary of the findings in Section 6. Appendix A provides proofs for some of the results of the paper.

2. Setting the stage

We follow the examples of Reid and Williamson (2011), Zhao et al. (2013) and others in studying the subject of this paper at population level – as opposed to sample level. For the reason to do so, see Zhao et al. (2013) who state in Section 2.2 ‘To remove finite sample effects, we consider a data set of infinite size and hence the asymptotic expressions of error rate and balanced error rate.’ Refer also to Appendix B.1 of Zhao et al. (2013) for their rationale to deploy measure-theoretic formalism to classification problems.

2.1. Notation and setting

We use the following population-level description of the binary classification problem. See standard textbooks on probability theory like Bauer (1996) for formal definitions and background of the notions introduced in Assumption 2.1.

Assumption 2.1. $(\Omega, \mathcal{A}, P)$ is a probability space. An event $A \in \mathcal{A}$ with $0 < P[A] < 1$ and a sub-$\sigma$-field $\mathcal{H} \subset \mathcal{A}$ with $A \notin \mathcal{H}$ are fixed.

Interpretation

- The elements $\omega$ of $\Omega$ are objects (or instances) with class and feature properties. $\omega \in A$ means that $\omega$ belongs to class 1 (or the positive class). $\omega \in A^c = \Omega \setminus A$ means that $\omega$ belongs to class 0 (or the negative class).
- The $\sigma$-field $\mathcal{A}$ of events $M \in \mathcal{A}$ is a collection of subsets $M$ of $\Omega$ with the property that they can be assigned probabilities $P[M]$ in a logically consistent way.
- Binary classification problem: The sub-$\sigma$-field $\mathcal{H} \subset \mathcal{A}$ contains the events which are observable at the time when the class of an object $\omega$ has to be predicted. Since $A \notin \mathcal{H}$, then the class of an object is not known. It can only be inferred on the basis of the events $H \in \mathcal{H}$ which are assumed to reflect the features of the instance.

Reconciliation with the standard setting for binary classification in the machine learning and pattern recognition literature (see e.g. Devroye et al., 1996):

- Typically a random vector $(X, Y)$ is studied, where $X$ stands for the features of an instance and $Y$ stands for its class. $X$ is assumed to take values in a feature space $\mathcal{X}$ (often $\mathcal{X} = \mathbb{R}^d$) while $Y$ takes either the value 0 (or $-1$) or the value 1 (for the positive class).
• Standard formulation of the binary classification problem: Infer the value of $Y$ from $X$ or make an informed decision on the occurrence or non-occurrence of $Y = 1$ despite only being able to observe the values of $X$.

• This is captured by the measure-theoretic setting of Assumption 2.1: Assume that $X$ and $Y$ map $\Omega$ into $\mathbb{R}$ and $\{0, 1\}$ respectively. Choose $\mathcal{H} = \sigma(X)$ (the smallest sub-$\sigma$-field of $\mathcal{A}$ such that $X$ is measurable) and $A = \{Y = 1\} = \{\omega \in \Omega : Y(\omega) = 1\}$.

• Often no probability space is specified but only a sample $(x_1, y_1), \ldots, (x_n, y_n)$ of realisations of $(X, Y)$ is considered. Usually this sample is assumed to have been generated by i.i.d. drawings from some population distribution which may be identified with $(\Omega, \mathcal{A}, P)$ as described above.

2.2. Posterior class probabilities

The probability of $A$ conditional on $\mathcal{H}$ (or posterior probability of the positive class) $\Psi = P[A | \mathcal{H}]$ is a central concept for binary classification and related areas, for the following reasons:

• As a consequence of Proposition 2.4 below on the decomposition of the Brier Score into refinement and calibration loss, $\Psi$ is the best predictor of $A$ in the sense of minimising the mean squared error.

• ‘Thresholding’ $\Psi$ produces the Bayes classifiers which minimise the Bayes error and cost-sensitive Bayes error respectively (Van Trees, 1968, p. 27; Devroye et al., 1996, Theorem 32.4).

• More generally, thresholding $\Psi$ also represents the best basis for many decision criteria for label assignments (classification) based on the confusion matrix (Koyejo et al., 2014, Theorem 2).

• $\Psi$ is best for statistical tests and binary classification based on Neyman-Pearson criteria (Scott, 2019).

• $\Psi$ is an optimum solution to the bipartite ranking problem (Menon and Williamson, 2016, Proposition 63).

• From the perspective of practice, estimates of $\Psi$ may serve as plug-in classifiers (Devroye et al., 1996, Section 2.5).

We refer to Section 4.1 of Durrett (1996) for the formal definitions and properties of

• expectation $E[Z | \mathcal{H}]$ of a random variable $Z$ conditional on $\mathcal{H}$, and

• probability $P[A | \mathcal{H}]$ of $A$ conditional on $\mathcal{H}$ respectively.

In the machine learning literature, often the term posterior class probability rather than conditional probability is used to refer to $P[A | \mathcal{H}]$, as opposed to the prior probability $P[A]$ which in our setting would rather be called unconditional probability of $A$. For a more concise notation, in the following we will sometimes write $\Psi$ or $\Psi_H$ for $P[A | \mathcal{H}]$.

Remark 2.2 ($\Psi$ vs. $\eta$). In the machine learning and pattern recognition literature, the posterior class probability often is denoted by $\eta$. See for instance Section 2.1 of Devroye et al. (1996) who introduced it as ‘regression of $Y$ on $X$’. If the sub-$\sigma$-field $\mathcal{H}$ from Assumption 2.1 is generated by a features random vector $X$ with values in a measurable space $\mathcal{X}$, i.e. $\mathcal{H} = \sigma(X)$, then the factorisation lemma (Bauer, 1996, Section 15) implies $\Psi = P[A | \sigma(X)] = \eta(X)$ for some measurable function $\eta : \mathcal{X} \rightarrow [0, 1]$. This function $\eta$ is the posterior probability (or regression function) (Devroye et al., 1996) and many other authors are referring to. In this paper, the slightly different $\Psi$-concept is preferred because it helps avoiding frequent changes of variables in expectations and integrals.

2.3. The Brier score and its components

The Brier score is an important tool for the analysis and practice of binary classification:

• As shown below, the Brier score plays an important role in the theoretical analysis of estimators of the posterior class probability $\Psi$. 
• By its definition as a mean squared error, representations of the Brier score and its components sometimes can be directly deployed for parametric or non-parametric regression.

See Chapter 6 of Hand (1997) for further background information on the Brier score.

**Definition 2.3 (Brier score).** Under Assumption 2.1, the Brier score \( BS(Z) \) (with respect to the event \( A \)) of a square-integrable \( A \)-measurable random variable \( Z \) is defined as

\[
BS(Z) = E[(1_A - Z)^2],
\]

where \( 1_A \) with \( 1_A(\omega) = \begin{cases} 1, & \omega \in A \\ 0, & \omega \not\in A \end{cases} \) denotes the indicator function of \( A \).

**Proposition 2.4 (Decomposition of Brier score).** Denote by \( \Psi_H \) the probability of \( A \) conditional on \( H \). Assume \( Z \) is a square-integrable \( H \)-measurable random variable (interpreted as estimator of \( A \) or probabilistic classifier). Then \( BS(Z) \) can be represented as sum of refinement loss \( E[\Psi_H (1 - \Psi_H)] \) and calibration loss \( E[(\Psi_H - Z)^2] \):\[
BS(Z) = E[\Psi_H (1 - \Psi_H)] + E[(\Psi_H - Z)^2]. \tag{1a}
\]

Assume \( \mathcal{G} \) is another sub-\( \sigma \)-field of \( H \) such that \( \mathcal{G} \subset H \) and define \( \Psi_G = P[A | \mathcal{G}] \). If \( Z \) is \( \mathcal{G} \)-measurable then decomposition (1a) can be modified to

\[
BS(Z) = E[\Psi_H (1 - \Psi_H)] + E[(\Psi_H - \Psi_G)^2] + E[(\Psi_G - Z)^2]. \tag{1b}
\]

In particular, it holds that

\[
E[\Psi_G (1 - \Psi_G)] = E[\Psi_H (1 - \Psi_H)] + E[(\Psi_H - \Psi_G)^2]. \tag{1c}
\]

The term \( E[(\Psi_H - \Psi_G)^2] \) is called grouping loss.

**Proof.** Regarding (1a) a short computation yields

\[
E[(1_A - Z)^2] = E[(1_A - \Psi_H)^2] + 2E[(1_A - \Psi_H)(\Psi_H - Z)] + E[(\Psi_H - Z)^2]
\]

\[
= P[A] - 2E[1_A \Psi_H] + E[\Psi_H^2] + 2E[(P[A | H] - \Psi_H)(\Psi_H - Z)] + E[(\Psi_H - Z)^2]
\]

\[
= P[A] - E[\Psi_H^2] + E[(\Psi_H - Z)^2] + E[\Psi_H (1 - \Psi_H)] + E[(\Psi_H - Z)^2].
\]

(1b) follows by straightforward application of the tower property of conditional expectation:

\[
E[(\Psi_H - Z)^2] = E[(\Psi_H - \Psi_G)^2] + 2E[(\Psi_H - \Psi_G)(\Psi_G - Z)] + E[(\Psi_G - Z)^2]
\]

\[
= E[(\Psi_H - \Psi_G)^2] + E[(\Psi_G - Z)^2] + 2E[(E[\Psi_H | \mathcal{G}] - \Psi_G)(\Psi_G - Z)].
\]

(1c) immediately follows from combining (1a) and (1b).

Some comments on Proposition 2.4:

• Proposition 2.4 implies that the probability of \( A \) conditional on \( H \) is the best estimate of \( A \) given the information reflected by \( H \), in the sense of minimising the mean-squared error. Thus Proposition 2.4 provides an alternative characterisation of conditional probabilities.

• Hand (1997) dealt with the multi-class case of (1a) and called \( E[(1_A - Z)^2] + E[(1_{A^c} - (1 - Z))^2] = 2E[(1_A - Z)^2] \) Brier inaccuracy.
• In the context of binary classification, the Brier Score is sometimes simply referred to as mean squared error (Hernández-Orallo et al., 2012, Definition 8).

• Hand (1997), Section 6.5, called the term \( E[\Psi (1 - \Psi)] \) inseparability and the term \( E[(\Psi - Z)^2] \) imprecision.

• We follow Hernández-Orallo et al. (2012), p. 2841, with the terms refinement loss for \( E[\Psi (1 - \Psi)] \) and calibration loss for \( E[(\Psi - Z)^2] \) respectively.

• Kull and Flach (2014), p. 22, introduced the concept of ‘grouping loss’. With a view on the fact that the \( \sigma \)-fields \( \mathcal{H} \) and \( \mathcal{G} \) reflect information that is utilised for estimating the respective conditional probabilities of \( A \), it would also seem appropriate to call the term \( E[(\Psi_{\mathcal{H}} - \Psi_{\mathcal{G}})^2] \) information gap loss. Kull and Flach (2014) called the Brier score component \( E[(\Psi_{\mathcal{G}} - Z)^2] \) group-wise calibration loss.

• Note the following alternative representation of the refinement loss:

\[
E[\Psi (1 - \Psi)] = P[A](1 - P[A]) - \text{var}[\Psi] = \text{var}[1_A] - \text{var}[\Psi].
\]

(2)

\( \text{var}[1_A] = P[A](1 - P[A]) \) is called uncertainty while \( \text{var}[\Psi] \) is called resolution.

Minimisation of the refinement loss in general is a matter of feature selection which is comprehensively covered in the literature (Chandrashekar and Sahin, 2014). Similarly, once feature selection has been completed and resulted in a fixed \( \sigma \)-field \( \mathcal{H} \), reducing calibration loss by transforming scoring classifiers into estimators of the true posterior probabilities given the scoring classifiers is a topic treated extensively in the literature (for a survey see Kull et al., 2017, Section 1).

However, as already observed by Murphy and Winkler (1977), the fact that the group-wise calibration loss \( E[(\Psi_{\mathcal{G}} - Z)^2] \) vanishes does not necessarily imply that the entire calibration loss is zero because the grouping loss can still be positive. Kull and Flach (2014), p. 22, advised to ‘train a new model’ in order to reduce the grouping loss portion of the calibration loss. In this paper, we focus attention to the grouping loss and to some suggestions of how to avoid it in the first place.

2.4. Classifier calibration and grouping loss

We study the connection between the following two approaches to the problem of estimating \( \Psi = P[A | \mathcal{H}] \) under Assumption 2.1 (cf. also Menon et al., 2012, Sections 3.1 and 3.2):

1) Directly estimate \( P[A | \mathcal{H}] \) from the observed data. Most of the time, this is a hard problem requiring huge datasets, primarily due to the curse of dimensionality if one wants to exploit the full information available in \( \mathcal{H} \) since \( \mathcal{H} \) typically represents observations in a multidimensional space (see, for instance, Hand, 1997, Chapter 5).

2) Find a scoring classifier (Hernández-Orallo et al., 2011, Section 2.1) \( S \), i.e. a real-valued \( \mathcal{H} \)-measurable random variable, such that high values of \( S \) reflect strong confidence that \( A \) has occurred and low values reflect weak confidence that \( A \) has occurred. Such random variables are sometimes also called confidence scores in the literature (Roelofs et al., 2020). Then estimate \( \Psi_{\sigma(S)} = P[A | \sigma(S)] \).

This is an easier task because it basically means to perform regression on one real-valued variable. In the machine learning literature such estimation exercises are called calibration of \( S \) (Zadrozny and Elkan, 2001).

Approach 2 actually means post-processing the result of a previous supervised learning exercise, for instance learning a support vector machine (SVM) or any other binary classification method that outputs a scoring classifier. Approach 2 therefore refers to a procedure with two steps which, however, in general both are considered to be easier and more efficient than approach 1.

Assume that feature selection has resulted in a fixed maximum amount of usable information, measured by the \( \sigma \)-field \( \mathcal{H} \). Then the refinement loss component in (1a) is a constant and, at the same time, the theoretical minimum estimation error that can be achieved when predicting the positive class event \( A \) based on the information provided by \( \mathcal{H} \). Applying the direct approach 1 is equivalent to trying to minimise the calibration loss component \( E[(\Psi_{\mathcal{H}} - Z)^2] \) in (1a).
In contrast, the second step of approach 2—the calibration of $S$—is better described by (1b), with $G = \sigma(S)$. The minimum achievable estimation error (refinement loss) is the same as for approach 1 but the calibration procedure is dealing only with the calibration loss portion

$$E[(\Psi_G - Z)^2] = E[(\Psi_{\sigma(S)} - Z)^2].$$

Indeed, measuring the goodness of calibration in the shape of $E[(\Psi_{\sigma(S)} - Z)^2]$ is an active research area (see Roelofs et al., 2020 for a recent example).

As mentioned before, Kull and Flach (2014) identified the grouping loss as a factor that impacts the total calibration loss (‘instance-wise calibration loss’ in their words). Kull and Flach (2014) observed that

$$E[(\Psi_H - \Psi_{\sigma(S)})^2] = E[\text{var}[\Psi_H | \sigma(S)]].$$ (3)

They proposed a local regression approach for estimating $\text{var}[\Psi_H | \sigma(S)]$ (more precisely a so-called reliability map based on this conditional variance) as a measure of reliability of their estimate of $\Psi_{\sigma(S)}$ as substitute of $\Psi_H$. This reliability measure then was used to improve an estimator for multi-class posterior probabilities.

In the remainder of this paper, we

- revisit in Section 3 the concept of sufficiency and its relation to the property that the grouping loss completely vanishes,
- revisit in Section 4 probing prediction (Langford and Zadrozny, 2005) as a tool to reduce both components of the calibration loss at the same time, and also
- discuss in Section 5 the role Brier curves (Hernández-Orallo et al., 2011) could play in controlling the grouping error if sufficiency cannot be achieved.

### 3. Sufficiency

In this section, we define a concept of sufficiency which is appropriate for the context of binary classification. At first glance, it differs from the more familiar statistical sufficiency with respect to a parametrised family of distributions as defined for instance in Casella and Berger (2002). See Section 3.2 below for comments on the connections between ‘statistical sufficiency’ and sufficiency in the sense of the following Definition 3.1.

#### 3.1. Sufficiency and admissibility

Devroye et al. (1996), Definition 32.2, defined ‘sufficiency’ in terms of random variables $X$ and $Y$ and called a mapping $T$ with the image of $X$ as its domain a sufficient statistic if for ‘for any set $A$, $P\{Y \in A | T(X), X\} = P\{Y \in A | T(X)\}’. Their definition of sufficiency thus is a special case of the following definition, with $M = \sigma(Y)$, $H = \sigma(X)$, and $G = \sigma(T(X))$.

**Definition 3.1.** Let $(\Omega, \mathcal{A}, P)$ be a probability space and $\mathcal{M}$, $\mathcal{G}$ and $\mathcal{H}$ be sub-$\sigma$-fields of $\mathcal{A}$ such that $\mathcal{G} \subset \mathcal{H}$. Then $\mathcal{G}$ is sufficient for $\mathcal{H}$ with respect to $\mathcal{M}$ if for all $M \in \mathcal{M}$

$$P[M | H] = P[M | G].$$ (4)

**Remark 3.2.** Under Assumption 2.1, let $\Psi = P[A | H]$ as well as

$$\mathcal{G} = \sigma(\Psi) \text{ and } \mathcal{M} = \sigma(\{A\}) = \{\emptyset, \Omega, A, A^c\}.$$ (5)

Then it is easy to show that $\mathcal{G}$ is sufficient for $\mathcal{H}$ with respect to $\mathcal{M}$. In applications, most of the time $\sigma(\Psi) \subset \mathcal{H}$ will hold because $\Psi$ is one-dimensional while $\mathcal{H}$ is likely to be generated by a multi-dimensional random vector. Hence it is indeed noteworthy that (4) is true in this context.
As already observed by Van Trees (1968), page 29, Remark 3.2 reflects the fact that $\Psi = P[A \mid \mathcal{H}]$ captures all the information contained in $\mathcal{H}$ that is relevant for inference regarding the event $A$. Van Trees (1968) called this property sufficiency without referring to any specific definition of the term.

The question is debatable if the nesting condition $\mathcal{G} \subset \mathcal{H}$ should be part of a definition of sufficiency as in Definition 3.1. The author chose to include the condition because inclusion comes at no cost for the discussion of calibration, the main topic of this paper. Nonetheless, definitions of sufficiency without nesting can make sense in other contexts. In Section 3.2 below, we also discuss the more general approach to sufficiency by Bröcker (2009).

At first glance, Definition 3.1 might not appear to be very helpful when it comes to controlling the grouping loss as defined in Proposition 2.4. Indeed, under Assumption 2.1, Eq. (4) is true for $M = A$ if and only if the grouping loss $E[(\Psi_{\mathcal{H}} - \Psi_{\mathcal{G}})^2]$ vanishes. Hence, there is a condition for the grouping loss to be zero, but we have not yet got criteria for the condition to apply. So far, by Remark 3.2 we know that a sufficient sub-$\sigma$-field of $\mathcal{H}$ exists. But, given that $\Psi = P[A \mid \mathcal{H}]$ is elusive, that observation does not really help.

At this point, it is useful to recall the notion of cost-sensitive learning and the related extended notion of Bayes classifier – see Section 32.3 of Devroye et al. (1996) for the details. Theorem 32.4 of Devroye et al. (1996) suggests that study of the solutions to cost-sensitive classification problems could provide further information for the problem of estimating posterior class probabilities. For this purpose, we introduce the following definition.

**Definition 3.3.** Under Assumption 2.1, for $H \in \mathcal{H}$ and $t \in [0, 1]$ the cost-weighted mean loss $L(H, t)$ is defined as

$$L(H, t) = (1 - t)P[A \cap H^c] + tP[A^c \cap H].$$

The cost-weighted Bayes loss $L^*_H(t)$ is defined as

$$L^*_H(t) = \inf_{H \in \mathcal{H}} L(H, t) = L(\{P[A \mid \mathcal{H}] > t\}, t).$$

With the notation of Definition 3.3, sufficiency can be characterised as follows:

**Theorem 3.4.** Under Assumption 2.1, let $\mathcal{G}$ denote a sub-$\sigma$-field of $\mathcal{H}$ (hence $\mathcal{G} \subset \mathcal{H}$). With the cost-weighted Bayes loss $L^*_H(t)$ defined as in (6b), then $\mathcal{G}$ is sufficient for $\mathcal{H}$ with respect to $\sigma(\{A\})$ (or simply $A$) if and only if for all $t \in (0, 1)$

$$L^*_H(t) = L^*_G(t).$$

**(7)**

**Proof.** The implication ‘sufficiency $\Rightarrow$ (7)’ is obvious from (6b).

For the converse, assume that (7) is true for all $t \in (0, 1)$. For $t \in (0, 1)$ define $G(t) = \{P[A \mid \mathcal{G}] > t\}$. Then as a consequence of (7), Theorem 4.2 below implies that

$$E[(Z - P[A \mid \mathcal{H}]^2) \leq 2 \int_0^1 L(G(t), t) - L^*_H(t) dt = 0,$$

with $Z = \int_0^1 1_{(0, P[A \mid \mathcal{G}])}(t) dt = P[A \mid \mathcal{G}]$. This implies $P[A \mid \mathcal{H}] = P[A \mid \mathcal{G}]$. \hfill $\Box$

In Example 3.12 of Section 3.2 below, we show that for the implication ‘(7) $\Rightarrow$ sufficiency’ to be true, the nesting condition $\mathcal{G} \subset \mathcal{H}$ must be assumed to hold. Nesting of the $\sigma$-fields involved comes naturally if Theorem 3.4 is phrased in terms of a transformation $T$ of the features, as noted in the following corollary.

**Corollary 3.5.** In the setting of Theorem 3.4, assume there is a measurable mapping $T : (\Omega, \mathcal{H}) \rightarrow (\Omega_T, \mathcal{A}_T)$ and let $\mathcal{G} = \sigma(T)$. Then (7) is equivalent to each of the following two properties:

(i) $\sigma(T)$ (or just $T$) is sufficient for $\mathcal{H}$ with respect to $A$, i.e. it holds that $P[A \mid \mathcal{H}] = P[A \mid \sigma(T)]$.

(ii) There is a measurable function $G : (\Omega_T, \mathcal{A}_T) \rightarrow (\mathbb{R}, \mathcal{B}(\mathbb{R}))$ such $P[A \mid \mathcal{H}] = G(T)$.
Proof. The equivalence of (7) and (i) a special case of Theorem 3.4. The equivalence of (i) and (ii) is a
direct consequence of the factorisation lemma.

In Corollary 3.5, the statement ‘(7) ⇔ (i)’ is Theorem 32.6 of Devroye et al. (1996). The statement ‘(7)
⇔ (ii)’ is Theorem 32.5 of Devroye et al. (1996). Devroye et al. (1996) called the mapping $T$ admissible if
(7) holds with $G = \sigma(T)$ since such mappings can be applied to transform the features without changing
the achievable minimum mean loss.

Further criteria for sufficiency – in addition to Theorem 3.4 – are desirable as (7) might be hard if not
impossible to show in practice.

**Proposition 3.6.** In the setting of Corollary 3.5, assume that there are an $\mathcal{H}$-measurable real-valued
random variable $T$ and a strictly increasing and continuous function $F : (0, 1) \to I \subset \mathbb{R}$ (where I may
denote a finite or infinite open interval) such that for all $t \in (0, 1)$ it holds that

$$L^*_\mathcal{H}(t) = L(\{T > F(t)\}, t),$$

(8)

with $L^*_\mathcal{H}$ and $L$ as in Definition 3.3. Denote by $G$ the inverse function of $F$ (hence $G$ is also strictly
increasing and continuous). Then it follows that $P[A | \mathcal{H}] = G(T)$, and $T$ is sufficient for $\mathcal{H}$ with respect
to $A$.

*Proof.* Proposition 3.6 follows from Theorem 4.2 in the same way as Theorem 3.4.

Proposition 3.6 could serve as justification for the familiar assumption that a scoring classifier can be
mapped by a strictly increasing transformation to the posterior probability of the positive class (Zadrozny
and Elkan, 2001; Kull et al., 2017). However, this would require to have (8) satisfied to a reasonable degree.

A related criterion for sufficiency rather refers to the ranking of the instances provided by the scoring
classifier than to optimality with respect to the mean cost-sensitive loss.

**Proposition 3.7.** In the setting of Corollary 3.5, assume that the mapping $T$ is real-valued. Assume
furthermore that $T$ and the probability $P[A | \mathcal{H}]$ of $A$ conditional on $\mathcal{H}$ are strongly comonotonic, i.e. it
holds for all $\omega_1, \omega_2 \in \Omega$ that

$$T(\omega_1) < T(\omega_2) \iff P[A | \mathcal{H}](\omega_1) < P[A | \mathcal{H}](\omega_2).$$

Then $\sigma(T)$ (or just $T$) is sufficient for $\mathcal{H}$ with respect to $A$, i.e. it holds that $P[A | \mathcal{H}] = P[A | \sigma(T)]$.

*Proof.* Combining Proposition 4.5 of Denneberg (1994) and Proposition 2.3 (iii) of Denneberg and Maaß
(2006), we obtain the existence of a strictly increasing function $\varphi : \mathbb{R} \to \mathbb{R}$ such that $P[A | \mathcal{H}] = \varphi(T)$.
As monotonic functions are Borel measurable, sufficiency of $T$ follows by Corollary 3.5.

By Proposition 3.7, ‘Covariate Shift with Posterior Drift’, a special type of dataset shift introduced by
Scott (2019), can alternatively be defined by postulating that the posterior class probabilities on the
source and target domains are strongly comonotonic. As a consequence, the posterior probability of the
source domain is sufficient with respect to the positive class labels also on the target domain.

At first glance, Proposition 3.7 might appear encouraging with regard to the chance to identify sufficient
random variables $T$ because the comonotonicity criterion does not look too demanding. For instance,
Zadrozny and Elkan (2002), at the beginning of Section 1, expressed confidence that this is typically
achieved when learning classifiers: ‘Most supervised learning methods produce classifiers that output
scores $s(x)$ which can be used to rank the examples in the test set from the most probable member to the
least probable member of a class $c$. That is, for two examples $x$ and $y$, if $s(x) < s(y)$ then $P(c|x) < P(c|y)$.’

However, while this statement is very plausible for potential comonotonicity of a scoring classifier $T$ and
posterior class probabilities $P[A | \sigma(T)]$, it is much less plausible with regard to probabilities $P[A | \mathcal{H}]$
conditional on the full available information. Moreover, comonotonicity of two real-valued random vari-
ables $X_1, X_2$ implies that Kendall’s $\tau$ and Spearman’s rank correlation take the value one when being
applied to $X_1, X_2$ (see, for instance, Dennit and Dhaene, 2003). This might not be easy to achieve, given the elusive nature of $P[A \mid H]$.

Note also that under Assumption 2.1 finding a mapping $T$ that is comonotonic with $P[A \mid H]$ is equivalent to solving the bipartite ranking problem (Clémençon and Vayatis, 2009, Section 2.1).

### 3.2. Alternative notions of sufficiency

Adragni and Cook (2009) introduced in Definition 1.1 sufficiency in a setting of random variables rather than $\sigma$-fields. Talking about ‘sufficient dimension reduction’, they considered univariate random variables $Y$ and $\mathbb{R}^p$-valued random vectors $X$ and defined ‘A reduction $R : \mathbb{R}^p \to \mathbb{R}^q$, $q \leq p$, is sufficient if it satisfies one of the following three statements:

(i) inverse reduction, $X \mid (Y, R(X)) \sim X \mid R(X)$,
(ii) forward reduction, $Y \mid X \sim Y \mid R(X)$,
(iii) joint reduction $(X \perp Y) \mid R(X)$,

where $\perp$ indicates independence, $\sim$ means identically distributed and $A \mid B$ refers to the random vector $A$ given the vector $B$.

A sufficient forward reduction in the sense of Adragni and Cook (2009) is a sufficient statistic in the sense of Devroye et al. (1996) and hence a special case of Definition 3.1. With regard to the relationship between ‘inverse reduction’, ‘forward reduction’ and ‘joint reduction’, Adragni and Cook (2009) stated: ‘They are equivalent when $(Y, X)$ has a joint distribution.’ In addition, according to Section 1(b) of Adragni and Cook (2009), ‘If we consider a generic statistical problem and reinterpret $X$ as the total data $D$ and $Y$ as the parameter $\theta$, then the condition for inverse reduction becomes $D \mid (\theta, R) \sim D \mid R$ so that $R$ is a sufficient statistic. In this way, the definition of a sufficient reduction encompasses Fisher’s (1922) classical definition of sufficiency.’ Van Trees (1968) made on pages 34 and 35 a similar comment in the special context of binary classification (see also DeGroot and Fienberg, 1983, Theorem 2).

The following proposition shows that also in the more general measure-theoretic setting of this paper, there is a meaningful notion of ‘sufficient inverse reduction’ that is equivalent to Definition 3.1 of sufficiency if $G \subseteq H$. In Proposition 3.8, the events $M$ of the $\sigma$-field $\mathcal{M}$ play the role the parameters $\theta$ play in the classical Fisher concept of sufficiency and the values of the variable $Y$ play in the definition of inverse reduction of Adragni and Cook (2009).

### Proposition 3.8

Let $(\Omega, \mathcal{A}, P)$ be a probability space and assume that $\mathcal{G}, \mathcal{H}$ and $\mathcal{M}$ are sub-$\sigma$-fields of $\mathcal{A}$. With the notation $\mathcal{F}_1 \vee \mathcal{F}_2 = \sigma(\mathcal{F}_1 \cup \mathcal{F}_2)$ for $\sigma$-fields $\mathcal{F}_1$ and $\mathcal{F}_2$, then the following three statements are equivalent:

(i) For all $H \in \mathcal{H}$, it holds that $P[H \mid G \vee M] = P[H \mid G]$.
(ii) For all $M \in \mathcal{M}$, it holds that $P[M \mid G \vee H] = P[M \mid G]$.
(iii) For all $H \in \mathcal{H}$ and all $M \in \mathcal{M}$, it holds that

$$P[H \cap M \mid G] = P[H \mid G] P[M \mid G].$$

The proof of Proposition 3.8 is straightforward, by making use of the properties of conditional probabilities. To reconcile Proposition 3.8 with the notion of sufficient dimension reduction used by Adragni and Cook (2009), choose

$$\mathcal{M} = \sigma(Y), \quad \mathcal{H} = \sigma(X), \quad \mathcal{G} = \sigma(R(X)) \subseteq \mathcal{H}. \quad (9)$$

Then Proposition 3.8 (i) describes sufficient inverse reduction, (ii) generalises sufficient forward reduction by not requiring $G \subseteq H$, and (iii) is another way to express sufficient joint reduction.

For a better understanding of Proposition 3.8, it is helpful to think of $\mathcal{M}$ as a collection of events to be predicted and of $\mathcal{H}$ as the maximal collection of observable events the prediction can be based on. Regarding $\mathcal{G}$, the following three cases may be considered separately:
Case 1: \(G \subset \mathcal{H} \). Then Proposition 3.8 (ii) is equivalent to Definition 3.1, and we are in the situation of Section 3.1 above where aggregation of observations without loss of prediction quality is sought in order to facilitate computations.

Case 2: \(G \nsubseteq \mathcal{H} \). Then Proposition 3.8 does not provide much value because all three statements are obviously true as \(\mathcal{H} \) basically becomes redundant in the statements of the proposition. However, due to our interpretation of \(\mathcal{H} \) as maximal collection of observable events, in this case \(G \) may contain unobservable events. This would make it unfit to substitute for \(\mathcal{H} \). But instead \(G \) could replace \(M \) as regression target, thanks to the tower property:

\[
P[M \mid \mathcal{H}] = E[P[M \mid G] \mid \mathcal{H}].
\]

(10)

So-called shadow ratings are an example for this approach (Erlenmaier, 2011). Another example is the situation where weather forecasters \(G \) and \(\mathcal{H} \) have access to a common set of observation stations but deploy different meter-readers who make independent reading errors. Formally, an example for case 3 could be a situation with two weather forecasters. They might rely on the same observation stations but get extra data from some additional stations not in the common set.

Case 3: \(G \nsubseteq \mathcal{H} \) and \(\mathcal{H} \nsubseteq G \). Proposition 3.8 is non-trivial in this case. It is similar to case 2 in so far as again \(G \) may contain unobservable events. However, (10) is not automatically true in this situation but is implied by any of the equivalent statements of Proposition 3.8.

An example for case 3 could be a situation with two weather forecasters. They might rely on the same observation stations but deploy different meter-readers who make independent reading errors. Formally, this situation could be described as in the following example.

Example 3.9. Under Assumption 2.1, let \(G \) be a sub-\(\sigma\)-field of \(\mathcal{H} \) that is sufficient for \(\mathcal{H} \) with respect to \(A\) in the sense of Definition 3.1. Assume that \(I\) and \(J\) are further sub-\(\sigma\)-fields of \(A\) such that \(I \cup J\) and \(\mathcal{H} \cup \{\emptyset, \Omega, A, A^c\}\) are independent. Let \(G^* = G \cup I\) and \(\mathcal{H}^* = \mathcal{H} \cup J\). Then it follows that

\[
P[A \mid \mathcal{H}^* \cup G^*] = P[A \mid G^*],
\]

such that for \(G^*, \mathcal{H}^*\) and \(\mathcal{M} = \{\emptyset, \Omega, A, A^c\}\) statement (ii) of Proposition 3.8 is true. \(\square\)

Is the condition \(G \subset \mathcal{H}\) actually not needed in Definition 3.1? Would Theorem 3.4 still be true if Definition 3.1 were replaced by statement (ii) of Proposition 3.8 without requiring \(G \subset \mathcal{H}\)?

Indeed, Schervish (1989) (in Definition 10.1) and Bröcker (2009) (in Eq. (14)) defined sufficiency by means of (10), without requiring \(G \subset \mathcal{H}\) or \(\mathcal{H} \subset G\). Bröcker (2009) provided in Section 4 another non-trivial example for the third case we described above.

Theorem 10.2 of Schervish (1989) seems to suggest that Theorem 3.4 is true under (10) instead of sufficiency according to Definition 3.1. Below we show that Theorem 10.2 of Schervish (1989) needs to be carefully interpreted.

- In Proposition 3.10, we prove that indeed (10) implies \(L^*_G(t) \leq L^*_H(t)\) for the cost-weighted Bayes losses associated with \(G\) and \(\mathcal{H}\) respectively in the sense of Definition 3.3.

- However, in Example 3.3 we show that \(L^*_G(t) \leq L^*_H(t)\) for all \(t \in (0,1)\) does not always imply (10) (and therefore neither of the three statements of Proposition 3.8) if \(G \subset \mathcal{H}\) does not hold.

Proposition 3.10. Under Assumption 2.1, let \(G\) be another sub-\(\sigma\)-field of \(A\) and assume that (10) is true with \(M = A\). Then for all \(t \in (0,1)\) it holds that

\[
L^*_G(t) \leq L^*_H(t).
\]

(11)

Proof. Fix any \(H \in \mathcal{H}\) and \(0 < t < 1\). Then we obtain

\[
L(H, t) = (1 - t) P[A \cap H^c] + t P[A^c \cap H] = (1 - t) E[1_{H^c} P[A \mid \mathcal{H}] + t E[1_{H} (1 - P[A \mid \mathcal{H}])] = (1 - t) E[E[1_{H^c} P[A \mid G] \mid \mathcal{H}] + t E[1_{H} (1 - E[1_{H} P[A \mid G] \mid \mathcal{H}])] = (1 - t) E[(1 - P[H \mid G]) P[A \mid G] + t E[P[H \mid G] (1 - P[A \mid G])] = (1 - t) E[1_{A} (1 - P[H \mid G])] + t E[1_{A^c} P[H \mid G]].
\]

(12)
Closer inspection of Theorem 32.4 of Devroye et al. (1996) shows that it does not only apply to ‘decision functions’ but also to ‘randomised decision classifiers’ in the sense of Tasche (2018). Therefore, (12) implies $L(H, t) \geq L^*_G(t)$ and hence also (11).

Proposition 3.10 in conjunction with (15b) from Section 4.1 below implies that under (10) the refinement loss (in terms of the Brier score) of $\mathcal{G}$ is not greater than the refinement loss of $\mathcal{H}$ – which was proven by Bröcker (2009) for resolution and refinement defined in terms of general proper scores.

In order to show that (11) for all $t \in (0, 1)$ does in general not imply (10), we make use of the following lemma.

**Lemma 3.11.** Under Assumption 2.1, let $\mathcal{G}$ be another sub-$\sigma$-field of $\mathcal{A}$ such that $\mathcal{H}$ and $\mathcal{G}$ are independent conditional on $A$ and independent conditional on $A^c$. Assume $L^*_G(t) > 0$ for some $t \in (0, 1)$. Then (10) (with $M = A$) implies that $A$ and $\mathcal{H}$ are independent (hence $P[A | \mathcal{H}] = P[A]$ is constant).

**Proof.** For any $H \in \mathcal{H}$ we obtain

$$P[A \cap H] = E[1_H P[A | \mathcal{H}]] = E[1_H E[P[A | \mathcal{G}] | \mathcal{H}]] = E[1_H P[A | \mathcal{G}]] = P[A] E[1_H P[A | \mathcal{G}] | A] + P[A^c] E[1_H P[A | \mathcal{G}] | A^c] = P[A] P[H | A] E[P[A | \mathcal{G}] | A] + P[A^c] P[H | A^c] E[P[A | \mathcal{G}] | A^c].$$

This implies for all $H \in \mathcal{H}$

$$P[A] P[H | A] \left(1 - E[P[A | \mathcal{G}] | A]\right) = P[A^c] P[H | A^c] E[P[A | \mathcal{G}] | A^c].$$

Choosing $H = \Omega$ gives

$$P[A] \left(1 - E[P[A | \mathcal{G}] | A]\right) = P[A^c] E[P[A | \mathcal{G}] | A^c].$$

Then $E[P[A | \mathcal{G}] | A^c] = 0$ would imply $E[P[A | \mathcal{G}] | A] = 1$ (also vice versa) and hence $P[A | \mathcal{G}] = 0$ on $A^c$ and $P[A | \mathcal{G}] = 1$ on $A$, almost surely. From this it would follow that

$$L^*_G(t) = (1 - t) P[A \cap \{P[A | \mathcal{G}] \leq t\}] + t P[A^c \cap \{P[A | \mathcal{G}] > t\}] = 0,$$

contradicting the assumption $L^*_G(t) > 0$. Hence (13a) and (13b) imply

$$P[H | A] = P[H | A^c]$$

for all $H \in \mathcal{H}$.

In plain language, this means that $A$ and $\mathcal{H}$ are independent.

**Example 3.12.** Figure 1 shows curves $t \mapsto L^*_H(t)$ and $t \mapsto L^*_G(t)$ for $0 \leq t \leq 1$ for different choices of $\mathcal{H}$ and $\mathcal{G}$, with the cost-weighted Bayes loss $L^*_H(t)$ defined by (6b).

- For Figure 1, under Assumption 2.1 a model based on bivariate normal feature distributions with different mean vectors but identical covariance matrices has been chosen. The correlation between the components is assumed to be zero. Therefore the two components $X_1$ and $X_2$ of the normal distributions are independent conditional on the classes (i.e. given $A$ and $A^c$ respectively in the setting of Assumption 2.1). We define $\mathcal{H} = \sigma(X_1)$ and $\mathcal{G} = \sigma(X_2)$ such that $\mathcal{G} \not\subset \mathcal{H}$ and $\mathcal{H} \not\subset \mathcal{G}$.

- The dashed curve of Figure 1 shows the curve $t \mapsto L^*_H(t)$ of the true posterior class probability, making use of the full information available (i.e. both marginal components). Note that the maximum of this optimal curve is lower than the maximum of the optimal curve in Figure 2 below. This is due to the fact that for this example zero correlation between the components of class conditional distribution is assumed.
Figure 1: Illustration of Example 3.12. The conditional feature distributions are uncorrelated bivariate normal with identical covariance matrices. The prior probability of the positive class is 10%.

- The dotted curve shows \( t \mapsto L^*_H(t) \) (i.e. the curve for \( X_1 \), hence based on partial information only).
- The dash-dotted curve shows \( t \mapsto L^*_G(t) \) (i.e. the curve for \( X_2 \), also based on partial information only).
- The solid curve shows \( t \mapsto L^*_\{\emptyset, \Omega\}(t) = \min((1 - t) P[A], t (1 - P[A])) \), the curve for the constant ‘prior estimate’ \( P[A] \).

Clearly, the curve for \( X_2 \) is dominated by the curve for \( X_1 \), i.e. (11) is true for all \( t \in (0, 1) \). However, if \( \mathcal{G} = \sigma(X_2) \) and \( \mathcal{H} = \sigma(X_1) \) satisfied (10), by Lemma 3.11 \( X_1 \) and \( A \) would be independent. Hence we would have \( P[A \mid \sigma(X_1)] = P[A] \) constant and the curve for \( X_1 \) would be the solid curve. This is clearly not the case since the solid and the dotted curves do not coincide. It follows that (10) cannot be true for \( \mathcal{G} = \sigma(X_2) \) and \( \mathcal{H} = \sigma(X_1) \).

How to reconcile Example 3.12 with Theorem 10.2 of Schervish (1989)? Unfortunately, Schervish (1989) did not provide a detailed proof of the theorem but only suggested the building stones needed for a proof. Therefore it seems possible that in some of the steps of the proof an assumption would have to be made that forecaster A had no more information at her disposal than forecaster B (in terms of this paper: \( \mathcal{G} \subseteq \mathcal{H} \)). This way, Theorem 10.2 of Schervish (1989) would contradict neither Example 3.12 nor Theorem 3.4.

As observed in (Krüger and Ziegel, 2021, p. 974), according to Strassen’s theorem (Strassen, 1965), inequality (11) holds if and only if there are random variables \( Z_{\mathcal{G}} \) and \( Z_{\mathcal{H}} \) on a possibly different probability space such that

- the distributions of \( Z_{\mathcal{G}} \) and \( P[A \mid \mathcal{G}] \) are equal,
- the distributions of \( Z_{\mathcal{H}} \) and \( P[A \mid \mathcal{H}] \) are equal, and
- it holds that \( E[Z_{\mathcal{G}} \mid \sigma(Z_{\mathcal{H}})] = Z_{\mathcal{H}} \).
This observation does not contradict Example 3.12 because there we have shown that (10) does not hold almost surely (i.e. with probability 1). This does not exclude the possibility that equality holds in distribution.

4. Probing reduction

What if we do not find a sufficient scoring classifier $T$ for $H$, for instance when we cannot be sure to have reached the minimum on the left-hand side of (7), or when there are doubts that $T$ is comonotonic with $P[A \mid H]$? By Corollary 3.5, without sufficiency of $T$ the relation $P[A \mid H] = G(T)$ cannot be achieved. Is then everything lost if no sufficient scoring classifier can be identified?

The criteria for sufficiency we have presented in Section 3.1 have in common that they involve finding a single variable $T$ which solves an infinite number of optimisation problems at the same time, see for instance Proposition 3.6. This might be a difficult task. It would be nice to be able to separately solve the optimisation problems, resulting in a family of optimal classifiers, and then to combine the classifiers to one sufficient scoring classifier $T$ which provides the required simultaneous solution for all the optimisation problems.

Without referring to the notions of sufficiency or bipartite ranking, Langford and Zadrozny (2005) presented ‘probing reduction’ as a way to achieve this feat. They described their method with the statement ‘reduce learning an estimator of class probability membership [sic] to learning binary classifiers’. As part of their theoretical analysis, Langford and Zadrozny (2005) proved a theorem on ‘probing error transformation’ which implies the results of Devroye et al. (1996), Section 32.3, on sufficiency and admissibility and provides a constructive way to estimate posterior probabilities exploiting all the information available.

In the following, we present a slightly more abstract version of the ‘probing predictor’ and Theorem 2 of Langford and Zadrozny (2005).

4.1. Preliminaries

Under Assumption 2.1, let $Z$ be a real-valued $A$-measurable random variable. For $t \in [0, 1]$ and $\omega \in \Omega$ let

$$
\ell_Z(\omega, t) = (1 - t) \mathbf{1}_A(\omega) \mathbf{1}_{[Z(\omega), 1]}(t) + t \mathbf{1}_{A^c}(\omega) \mathbf{1}_{[0, Z(\omega))}(t).
$$

For fixed $\omega \in \Omega$, then $t \mapsto \ell_Z(\omega, t)$ is right-continuous on $[0, 1)$ and has left limits for $t \in (0, 1]$. As a consequence $\ell_Z(\omega, t)$ is jointly measurable in $(\omega, t)$, see any standard textbook on the theory of stochastic processes. Moreover, with $L(H, t)$ and $L^*_H(t)$ defined as in Definition 3.3, it holds that

$$
L\left(\{Z > t\}, t\right) = E[\ell_Z(\cdot, t)] \quad \text{and} \quad L^*_H(t) = E[\ell_\Psi(\cdot, t)],
$$

for $\Psi = P[A \mid H]$. The double integrals appearing in the following proposition therefore are well-defined. The result was shown by Hernández-Orallo et al. (2012), Theorem 14 and Theorem 29. It had been proven before by Langford and Zadrozny (2005) as part of their proof of Theorem 2. Thus the result is needed for the proof of Theorem 4.2 below but is also of interest of its own.

**Proposition 4.1.** Under Assumption 2.1, with the cost-weighted mean loss defined as in (6a) and the Brier score $BS$ as in Definition 2.3, for any $A$-measurable random variable $Z$ with values in $[0, 1]$ it holds that

$$
2 \int_0^1 L\left(\{Z > t\}, t\right) dt = BS(Z).
$$

With the cost-weighted Bayes loss defined as in (6b) and $\Psi = P[A \mid H]$, the refinement loss $E[\Psi (1 - \Psi)]$ (see Proposition 2.4) can be represented as

$$
2 \int_0^1 L^*_H(t) dt = E[\Psi (1 - \Psi)].
$$
Note that (15a) and (15b) differ from the statements in Theorem 14 and Theorem 29 respectively of Hernández-Orallo et al. (2012) by the factor $1/2$ being applied to the Brier score on the right-hand side. This is a consequence of Hernández-Orallo et al. (2012) having scaled the Bayes error terms by the factor $2$.

**Proof of Proposition 4.1.** Starting from the left-hand side of (15a), we obtain by making use of (14b) and Fubini’s theorem

\[
\int_0^1 L(\{Z > t\}, t) \, dt = \int_0^1 E[\ell_Z(\cdot, t)] \, dt \\
= E \left[ 1_A \int_Z (1 - t) \, dt + 1_{A^c} \int_0^t \, dt \right] \\
= E[1_A (1 - Z)^2/2 + 1_{A^c} Z^2/2].
\]

Observing that $1_A (1 - Z)^2 + 1_{A^c} Z^2 = (1_A - Z)^2$ implies (15a). Eq. (15b) follows by combining (15a) and (1a) (with $Z = \Psi$).

\[ \square \]

### 4.2. Main result

The following theorem basically is a restatement of Theorem 2 of Langford and Zadrozny (2005), with some changes to the notation and a different representation of the ‘probing predictor’ in (16a). See also Remark 4.3 below for more details on how Theorem 4.2 differs from the original version given by Langford and Zadrozny (2005).

**Theorem 4.2.** Under Assumption 2.1, define the cost-weighted mean loss $L(H, t)$ and the cost-weighted Bayes loss $L^*_H(t)$ for $H \in \mathcal{H}$ and $0 \leq t \leq 1$ as in Definition 3.3. Assume that for each $t \in (0, 1)$ a classifier represented by $H(t) \in \mathcal{H}$ is given such that the function $h: (0, 1) \times \Omega \to \{0, 1\}$ with

\[
h(t, \omega) = \begin{cases} 
1, & \text{if } \omega \in H(t), \\
0, & \text{if } \omega \notin H(t),
\end{cases}
\]

is $\mathcal{B}((0, 1)) \otimes \mathcal{H}$-measurable. Define the $\mathcal{H}$-measurable random variable $Z$ by

\[
Z(\omega) = \int_0^1 h(t, \omega) \, dt.
\]

Let $\Psi = P[A | \mathcal{H}]$. Then it follows for the calibration loss $E[(Z - \Psi)^2]$ of $Z$ that

\[
E[(Z - \Psi)^2] = 2 \int_0^1 L(\{Z > t\}, t) - L^*_H(t) \, dt \\
\leq 2 \int_0^1 L(H(t), t) - L^*_H(t) \, dt
\]

See Appendix A.1 for a proof of Theorem 4.2.

**Remark 4.3.** Comments on Theorem 4.2:

1) Actually, Langford and Zadrozny (2005) proved in Theorem 2 the following version of Theorem 4.2 (rephrased in the notation of this paper):

With the notation $\bar{L}(H, t) = \frac{1}{N_t} P[A \cap H^c] + P[A^c \cap H]$ and $N_t = \frac{1}{1-t} P[A] + P[A^c]$ for $t \in (0, 1)$, it holds that

\[
E[(Z - \Psi)^2] \leq 2 \max(P[A], 1 - P[A^c]) \int_0^1 \bar{L}(H(t), t) - \bar{L}((\Psi > t), t) \, \frac{dt}{N_t}.
\]

14
Observing that $t N_t \leq \max(P[A], 1 - P[A])$, one finds that
\[
\max(P[A], 1 - P[A]) \int_0^1 \frac{\bar{L}(H(t), t) - \bar{L}(\{\Psi > t\}, t)}{N_t} \, dt \\
\geq \int_0^1 t (\bar{L}(H(t), t) - \bar{L}(\{\Psi > t\}, t)) \, dt \\
= \int_0^1 L(H(t), t) - L^*_H(t) \, dt.
\]

At first glance, therefore, the upper bound for $E[(Z - \Psi)^2]$ of Theorem 2 of Langford and Zadrozny (2005) is less strict than the upper bound provided by Theorem 4.2. However, a closer inspection of the proof of Theorem 2 of Langford and Zadrozny (2005) reveals that they indeed proved (16b) but due to their different notion of approximation error ended up in stating an apparently weaker result. With a view to applications, however, $\bar{L}(H, t)$ reflects the fact that the weight-dependent classifiers from the right-hand side of (16a) likely would be trained on samples in which only one class is re-weighted – not on samples with both classes re-weighted as suggested by definition (6a) of $L(H, t)$.

2) The ‘probing predictor’ $\hat{p}(x)$ of Langford and Zadrozny (2005) (which corresponds to $Z$ in the notation of this paper) is obtained by ‘sort[ing] the results of the classifiers to make the sequence monotonic (all zeroes before all ones)’. Defining $Z$ as the average of the $h(t, \cdot)$ has the same effect as sorting but has the advantage to be viable also in the infinite sample case of this paper.

3) Langford and Zadrozny (2005) commented on their Theorem 2 as follows: ‘This is a strong theorem in the sense that it ties the error in the probability predictions to the average relative importance weighted loss of the classifiers. Using the average loss over $w$ [in the notation of this paper] results in a more powerful statement than using the maximal loss, because it is easier to obtain a set of classifiers which have small average loss than to obtain a set of classifiers, all with a small loss. Using a loss that is relative to the loss of the Bayes optimal classifier means that the theorem applies even when the fundamental noise rate is large.’

4) In addition to the comment of Langford and Zadrozny (2005) on the theorem as quoted in 3), it might be worthwhile to point out that the ‘probing predictor’ $\hat{p}(x)$ (or $Z$ in the notation of this paper) performs better on average than the classifiers $H_t$, $0 < t < 1$ that are the input to the estimation procedure (besides the data). This is clearly stated in Theorem 4.2 above but was implicitly stated already in the proof of Theorem 2 of Langford and Zadrozny (2005).

The following example illustrates how (16a) can be used to combine two estimators $Z_1$ and $Z_2$ of the posterior class probability $P[A | H]$ to form another estimator $Z$ with a potentially smaller Brier score.

**Example 4.4.** Let $Z_1, Z_2$ be $\mathcal{H}$-measurable random variables with values in $[0, 1]$ and let $0 < z < 1$ be fixed. Define
\[
Z = \int_0^z 1_{\{Z_1 > t\}} \, dt + \int_z^1 1_{\{Z_2 > t\}} \, dt \\
= \min(z, Z_1) + (Z_2 - z) 1_{\{Z_2 > z\}}.
\]

If $z$ is chosen in such a way that
\[
L(\{Z_1 > t\}, t) \leq L(\{Z_2 > t\}, t) \quad \iff \quad t \leq z,
\]
then by (16b) it follows that
\[
BS(Z) \leq \min(BS(Z_1), BS(Z_2)).
\]

Such a number $z$ could be identified by inspection of the Brier curves of $Z_1$ and $Z_2$, see for example the criss-crossing dashed and dash-dotted curves in Figure 2 below.
5. **Brier curves**

The name and notion of Brier curves as discussed in this section were introduced by Hernández-Orallo et al. (2011). At about the same time, the concept was considered by Reid and Williamson (2011) who called it ‘risk curves for costs’. However, such curves – without being given specific names – were presented much earlier in the literature (see Ehm et al., 2016, p. 519, for more details).

5.1. **Definition and properties**

**Definition 5.1 (Brier curve).** For a probabilistic classifier $Z$ (i.e. an $\mathcal{H}$-measurable $[0,1]$-valued random variable), the Brier curve $t \mapsto B(t)$ is defined as

$$B(t) = L(\{Z > t\}, t), \quad t \in [0,1],$$

where $L(\cdot,t)$ denotes the cost-weighted mean loss of Definition 3.3.

The definition of Brier curve used here differs from the definition in Eq. (10) of Hernández-Orallo et al. (2011) by a factor 2. By multiplying with 2, one would achieve equality between the area under the Brier curve and the Brier score (see comments below). The ‘Brier curve for skew’ as defined in Eq. (11) of Hernández-Orallo et al. (2011) is just the Brier curve as in Definition 5.1 (but scaled with factor 2).

By Proposition 4.1, the Brier score for $Z \mapsto P[Z \leq t | A]$ and $t \mapsto P[Z \leq t | A^c]$, the Brier curve for $Z$ can be represented as

$$B(t) = (1 - t) P[A] P[Z \leq t | A] + t (1 - P[A]) (1 - P[Z \leq t | A^c]), \quad 0 \leq t \leq 1. \quad (18)$$

- By (18), $t \mapsto B(t)$ is right-continuous on $[0,1)$ and has left limits for all $t \in (0,1]$.
- $B(t) \geq 0$ for all $t \in [0,1]$, $B(1) = 0$, $B(0) = P[A] P[Z = 0 | A]$.
- Denoting by $B_Z(t)$, $B_{Z^c}(t)$ and $B_{\Psi}(t)$ the Brier curves of a probabilistic classifier $Z$, of its calibrated version $Z^* = P[A | \sigma(Z)]$, and of the posterior probability $\Psi = P[A | \mathcal{G}]$ respectively, it holds that

$$B_Z(t) \geq B_{Z^c}(t) \geq B_\Psi(t), \quad t \in [0,1]. \quad (19)$$

- By Proposition 4.1, the Brier score for $Z$ equals twice the area below the Brier curve of $Z$.
- If both conditional distributions $P[Z \in \cdot | A]$ and $P[Z \in \cdot | A^c]$ have continuous Lebesgue densities $g_A$ and $g_{A^c}$ respectively, then the Brier curve $B(t)$ of $Z$ is continuously differentiable in $(0,1)$ with

$$\frac{dB}{dt}(t) = 1 - P[A] - P[Z \leq t] + (1 - t) P[A] g_A(t) - t (1 - P[A]) g_{A^c}(t). \quad (20)$$

The following proposition not only applies to the ‘full information’ posterior probability $\Psi = P[A | \mathcal{G}]$, but also to any calibrated probabilistic classifier $Z = P[A | \sigma(Z)]$ (case $\mathcal{G} = \sigma(Z)$).

**Proposition 5.2 (Properties of Brier curves for calibrated probabilistic classifiers).** Under Assumption 2.1, let $\mathcal{G}$ denote some sub-$\sigma$-field of $\mathcal{H}$ and define $\Psi = P[A | \mathcal{G}]$. Then the Brier curve $t \mapsto B(t)$ of $\Psi$ according to Definition 5.1 has the following properties:

1) $B$ is concave and continuous on $[0,1]$, with $B(0) = 0$.

2) For all $0 \leq t \leq 1$, it holds that

$$\min(t, 1 - t) E[\Psi (1 - \Psi)] \leq B(t) \leq E[\Psi (1 - \Psi)]. \quad (21)$$
3) In (21), we have \( \min(t, 1-t) E[\Psi(1-\Psi)] = B(t) \) if and only if \( \Psi \) is constant with \( P[A] = 0 = \Psi \) or \( P[A] = 1 = \Psi \). On the right-hand side of (21), it holds that \( B(t) = E[\Psi(1-\Psi)] \) if and only if \( \Psi \) is constant with \( P[A] = t = \Psi \).

4) \( B \) has for each \( t \in [0,1) \) the right derivative \( \frac{d}{dt}B(t) = 1 - P[A] - P[\Psi \leq t] \) and for each \( t \in (0,1] \) the left derivative \( \frac{d}{dt}B(t) = 1 - P[A] - P[\Psi < t] \).

5) We call, for a real-valued random variable \( Z \) and \( \alpha \in (0,1) \), any number \( z \) with \( P[Z < z] \leq \alpha \leq P[Z \leq z] \) an \( \alpha \)-quantile of \( Z \). Then for all \((1 - P[A])-\)quantiles \( t^* \) of \( \Psi \) it holds that

\[
\max_{0 \leq t \leq 1} B(t) = B(t^*).
\]

6) Assume there is another probability measure \( Q \) on \( (\Omega, \mathcal{A}) \) such that \( Q \) and \( P \) are related through prior probability shift on \( \mathcal{G} \), i.e. for some \( p, q \in (0,1) \) it holds that

\[
q = Q[A] \neq P[A] = p, \text{ as well as } Q[G|A] = P[G|A] \text{ and } Q[G|A^c] = P[G|A^c], \quad G \in \mathcal{G}.
\]

Let \( \Psi_Q = Q[A|\mathcal{G}] \) and \( \Psi_P = P[A|\mathcal{G}] \), and define for \( t \in [0,1] \):

\[
B_Q(t) = (1-t)Q[A \cap \{ \Psi_Q \leq t \}] + tQ[A^c \cap \{ \Psi_Q > t \}], \quad \text{and} \quad B_P(t) = (1-t)P[A \cap \{ \Psi_P \leq t \}] + tP[A^c \cap \{ \Psi_P > t \}].
\]

Then it follows that

\[
\frac{B_Q(t)}{(1-t)q} = \frac{B_P(s)}{(1-s)p}, \quad 0 < t < 1,
\]

with \( s = \frac{(1-q)pt}{(p-q)t+q(1-p)} \).

See Appendix A.2 for a proof of Proposition 5.2.

- (21) generalises Theorem 1 of Cohen and Goldszmidt (2004) from Bayes error to cost-weighted Bayes loss. Zhao et al. (2013) presented a general entropy-inspired approach to inequalities for the cost-sensitive error (21) can also be derived from inequality (31) of Zhao et al. (2013).

- Compare Proposition 5.2, item 4 to (20). Item 4 applies in full generality under Assumption 2.1 while for (20) the existence of continuous Lebesgue densities for the conditional feature distributions is needed. If this condition is satisfied then the comparison implies that (in the notation of (20)) the following equation is necessary for the probabilistic classifier to be calibrated:

\[
(1-t)P[A]g_A(t) = t(1-P[A])g_{A^c}(t), \quad 0 < t < 1.
\]

- Proposition 5.2, item 6 shows that Brier curves for true posterior class properties can easily be transformed into each other as long as the underlying distributions \( Q \) and \( P \) differ only by prior probability shift. Hence, in principle, for studying the properties of Brier curves for calibrated probabilistic classifiers, it suffices to look at the case \( P[A] = 1/2 \).

- Proposition 5.2, item 5 motivates Proposition 5.5 below with potentially useful bounds for the refinement loss related to \( \Psi = P[A|\mathcal{G}] \).

**Remark 5.3.** In the setting of Proposition 5.2, the problem to compute the value of the Brier curve for \( \Psi \) at \( t \in (0,1) \) (or equivalently the cost-weighted Bayes loss of (6b)) can be treated as a problem to determine an (unweighted) Bayes error, by making use of the following easy to prove relation:

\[
B(t) = \left( (1-t)P[A] + t(1-P[A]) \right) \min_{G \in \Psi} \left( qP[G^c|A] + (1-q)P[G|A^c] \right), \quad \text{with} \quad q = \frac{(1-t)P[A]}{(1-t)P[A] + t(1-P[A])}.
\]
Conversely, also the unweighted Bayes error can be determined by solving an optimisation problem for a cost-weighted mean loss (or determining a value on a Brier curve):

$$\min_{\alpha \in [0,1]} \left( P[A \cap G_c] + P[A^c \cap G] \right) = 2B_Q(1 - P[A]).$$  \hspace{1cm} (24b)

Here, the notation $B_Q$ indicates that the value of the Brier curve is determined for a probability measure $Q$ such that the prior probability of $A$ under $Q$ is $Q[A] = 1/2$.

**Remark 5.4.** By making use of (24a) and (24b), one can deploy Theorem 21 of Reid and Williamson (2011) to derive a representation of the Brier curve for $\Psi$ as in Proposition 5.2 in terms of the power function $\beta(\alpha)$ of the Neyman-Pearson test at size $\alpha$ based on the ratio of the densities of $P[G | A]$ and $P[G | A^c]$, $G \in G$, and vice versa:

$$B(t) = \left( (1 - t) P[A] + t (1 - P[A]) \right) \min_{\alpha \in [0,1]} \left( (1 - q) \alpha + q (1 - \beta(\alpha)) \right),$$  \hspace{1cm} (25a)

and

$$\beta(\alpha) = \inf_{p \in [0,1]} \frac{(1 - p) \alpha + p - 2B_Q(1 - p)}{p},$$  \hspace{1cm} (25b)

where the notation $B_Q$ indicates that the value of the Brier curve is determined for a probability measure $Q$ such that the prior probability of $A$ under $Q$ is $Q[A] = 1/2$ (as for (24b)). See Section 6 of Reid and Williamson (2011) for more information on the relationship between risk curves for costs, so-called risk curves for priors, and ROC curves.

The lower bound for the refinement loss component of the Brier score (see Proposition 2.4 above) in the following result is inspired by Proposition 5.2, item 5 and is a consequence of Proposition 5.2, item 2.

**Proposition 5.5.** Under Assumption 2.1, denote the probability of $A$ conditional on $\mathcal{H}$ by $\Psi = P[A | \mathcal{H}]$. Assume that there is a number $q \in [0,1]$ with $P[\Psi \leq q] = 1 - P[A]$. Then the following bounds apply for the refinement loss $E[\Psi (1 - \Psi)]$:

$$1 - \text{corr}[1_A, 1_{\{\Psi > q\}}] \leq \frac{E[\Psi (1 - \Psi)]}{P[A]} \leq 1 - \text{corr}[1_A, 1_{\{\Psi > q\}}]^2. \hspace{1cm} (26)$$

See Appendix A.3 for a proof of Proposition 5.5.

In Proposition 5.5, $1_{\{\Psi > q\}}$ is a moment-matching estimator of $1_A$ (same expected value and variance). If $\Psi$ is not exactly known but there is a scoring classifier $S$ (i.e. a $\mathcal{H}$-measurable random variable) which is strongly comonotonic with $\Psi$ then the event $\{\Psi > q\}$ can be replaced by $\{S > q^*\}$ where $q^*$ denotes a $(1 - P[A])$-quantile of $S$. Thus bounds for the refinement loss could be determined without exact knowledge of $\Psi$.

### 5.2. Application

In this section, based on the observations made before, we suggest:

- what can be done to avoid or at least control the grouping (or information gap) loss when estimating posterior class probabilities, and
- how this can be supported by the use of Brier curves.

In Figure 2, Brier curves are used to illustrate the decomposition of the Brier score as defined in Proposition 2.4 and the concept of grouping loss in particular.

- For Figure 2, a model based on bivariate normal feature distributions with different mean vectors but identical covariance matrices has been chosen. The two components of the normal distributions are positively correlated.
• The solid curve shows the Brier curve of the true posterior class probability, making use of the full information available (i.e. both marginal components and their correlation). The area under this curve is half of the optimal Brier score for the model and, therefore, also equals half of the refinement loss (or irreducible loss) associated with the model.

• The dash-dotted curve shows the Brier curve of a ‘partial’ posterior class probability, making use of only part of the available information (the first component of the normal distributions). The area between this curve and the solid curve equals half of the calibration loss, i.e. the Brier score for the partial posterior class probability minus the refinement loss for the model. In this case, the calibration loss is identical to the grouping loss because the partial posterior class probability is perfectly calibrated given the available information in the shape of the first component only.

• The dashed curve shows the Brier curve of a misspecified posterior class probability where the same formulae have been applied as for the true ‘full’ posterior class probability but with correlation set to zero. This corresponds to the naïve Bayes approach to the estimation of the posterior class probability and results in a poorly calibrated estimate. In this case, both components of the calibration loss as described in (1b) are positive.

• The dotted curve shows the Brier curve of the perfectly calibrated posterior class probability resulting from the naïve Bayes approach. While the correlation here is taken into account for the calibration, its misspecification in the design of the naïve Bayes score still results in an information gap (grouping loss) that is reflected in the area between the dotted curve and the solid curve. The area between the dotted and dashed curves is the calibration loss component due to using a misspecified formula for calibrating the naïve Bayes score underlying the dashed curve (this is called ‘group-wise calibration loss’ in Kull and Flach, 2014).

Recall that in the context of approach 2 of Section 2.4 to the estimation of posterior class probabilities we are dealing with a hierarchy of scoring classifiers (under Assumption 2.1):
• Scoring classifier (Hernández-Orallo et al., 2011): $\mathcal{H}$-measurable random variable $S : \Omega \rightarrow \mathbb{R}$.
• Probabilistic classifier (Hernández-Orallo et al., 2011): $\mathcal{H}$-measurable random variable $Z : \Omega \rightarrow [0,1]$, interpreted as estimator of posterior class probability $\Psi = P[A|\mathcal{H}]$.
• Calibrated probabilistic classifier: $\mathcal{H}$-measurable random variable $Z : \Omega \rightarrow [0,1]$ with the property $Z = P[A|\sigma(Z)]$. Hernández-Orallo et al. (2012) called in Definition 38 such probabilistic classifiers ‘perfectly calibrated’.
• True posterior class probability $\Psi = P[A|\mathcal{H}]$: In the terms introduced before in this paper, it can also be described as a sufficient, calibrated and probabilistic classifier.

Typically, a scoring classifier $S$ will be the outcome of some kind of optimisation procedure in the course of which one tries to link $S$ as best as possible to the positive class $A$, on the basis of a pre-defined set of features. This procedure commonly is described as ‘learning a classifier’ and can result in a scoring classifier with an arbitrary range (like in the case of SVMs) or in a probabilistic classifier (like in the case of binary logistic regression).

A number of efficient methods were proposed in the literature to deal with the problem of transforming a scoring or probabilistic classifier into a calibrated classifier (see Kull et al., 2017, and the references therein). However, focussing on this step only would fail to control the grouping loss.

5.3. Recommendation

Theorem 3.4 shows that the optimisation criterion for learning a scoring classifier $S$ must be carefully chosen in order to make sure that $S$ becomes sufficient for the full information content of $\mathcal{H}$ with respect to $A$. Only then the grouping loss for the estimation of the true posterior class probability will vanish. Proposition 3.6 suggests a way to achieve this: Show that $S$ satisfies (8) if not for all $t \in (0,1)$ then at least for a large number of $t$ that exhausts the whole interval $(0,1)$. This exercise can be supported by inspection of the Brier curve for $S$ constructed by plotting the right-hand side of (8) against $t$. This Brier curve should be concave and dominated by the Brier curves of all other candidate scoring classifiers.

By Remark 5.4, instead of striving to find the minimal Brier curve, equivalently we could try to find a scoring classifier $S$ such that the associated ROC curve is maximal (see, e.g., Marrocco et al., 2008). This observation provides additional support for the ‘ranking loss + isotonic regression’ approach proposed by Menon et al. (2012).

Recall also that Theorem 4.2 provides a promising alternative approach for combining optimal classifiers to obtain well-performing estimators of the posterior class probability. See Langford and Zadrozny (2005) for a practical implementation of this approach. What makes this approach particularly attractive is the fact that the classifiers being combined need not belong to the same type (e.g. SVMs) but can be chosen at discretion.

6. Conclusions

We have pointed out ‘grouping loss’ as a potentially contributing factor to the miscalibration of probabilistic classifiers. Grouping loss is caused by a gap between the information available for the calibration and the information actually taken into account for the calibration exercise. The absence of grouping loss is equivalent to the property of sufficiency as defined in Section 32.3 of Devroye et al. (1996) and known from statistics and the literature on dimension reduction techniques. Sufficiency in turn can be characterised in terms of the information needed for optimally solving a range of cost-weighted mean loss problems. We have presented further criteria for sufficiency like comonotonicity which might be easier to establish. In addition, we have presented an example that shows that ‘nesting’ as part of the definition of sufficiency is necessary for fully benefiting from the concept.

Nonetheless, in practice it could be difficult or even impossible to identify a sufficient scoring classifier. In this case, the so-called probing reduction (Langford and Zadrozny, 2005) might be useful. We have
restated the theorem that justifies this approach in order to better describe its connection to sufficiency and grouping loss.

Finally we have revisited the so-called Brier curves (Reid and Williamson, 2011; Hernández-Orallo et al., 2011) and provided an extensive list of their properties. Thanks to the fact that the area under a Brier curve for a probabilistic classifier is just half of the Brier score of that classifier, Brier curves are a useful tool for analysing calibration questions and can complement or even replace ROC curves in this respect as well as a criterion for classifier development.

**Acknowledgements**

The author thanks Tilmann Gneiting and an anonymous reviewer for suggestions that helped to improve earlier versions of this paper.

**References**

K.P. Adragni and R.D. Cook. Sufficient dimension reduction and prediction in regression. *Philosophical Transactions of the Royal Society A*, 367:4385–4405, 2009.

H. Bauer. *Probability Theory*. Walter de Gruyter, 1996.

B. Böken. On the appropriateness of Platt scaling in classifier calibration. *Information Systems*, 95:101641, 2021.

J. Bröcker. Reliability, sufficiency, and the decomposition of proper scores. *Quarterly Journal of the Royal Meteorological Society*, 135(643):1512–1519, 2009.

G. Casella and R.L. Berger. *Statistical Inference*. Duxbury Press, second edition, 2002.

G. Chandrashekar and F. Sahin. A survey on feature selection methods. *Computers & Electrical Engineering*, 40:16–28, 2014. doi: https://doi.org/10.1016/j.compeleceng.2013.11.024.

S. Clémençon and N. Vayatis. Tree-Based Ranking Methods. *IEEE Transactions on Information Theory*, 55(9):4316–4336, 2009.

I. Cohen and M. Goldszmidt. Properties and Benefits of Calibrated Classifiers. In *Proceedings of the 8th European Conference on Principles and Practice of Knowledge Discovery in Databases*, PKDD ’04, pages 125–136, Berlin, Heidelberg, 2004. Springer-Verlag.

M.H. DeGroot and S.E. Fienberg. The Comparison and Evaluation of Forecasters. *Journal of the Royal Statistical Society: Series D (The Statistician)*, 32(1/2):12–22, 1983. doi: https://doi.org/10.2307/2987588.

D. Denneberg. *Non-additive measure and integral*. Kluwer Academic Publishers, 1994.

D. Denneberg and S. Maas. Contribution values for allocation of risk capital and for premium calculation. Preprint, February 2006.

M. Denuit and J. Dhaene. Simple characterizations of comonotonicity and countermonotonicity by extremal correlations. *Belgian Actuarial Bulletin*, 3:22–27, 2003.

L. Devroye, L. Györfi, and G. Lugosi. *A Probabilistic Theory of Pattern Recognition*. Springer, 1996.

R. Durrett. *Probability: Theory and Examples*. Duxbury Press, second edition, 1996.

W. Ehm, T. Gneiting, A. Jordan, and F. Krüger. Of quantiles and expectiles: consistent scoring functions, Choquet representations and forecast rankings. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 78(3):505–562, 2016.
U. Erlenmaier. The Shadow Rating Approach: Experience from Banking Practice. In B. Engelmann and R. Rauhmeier, editors, The Basel II Risk Parameters, chapter 4, pages 37–74. Springer, second edition, 2011.

R.A. Fisher. On the Mathematical Foundations of Theoretical Statistics. Philosophical Transactions of the Royal Society of London, Series A, 222:309–368, 1922.

D.J. Hand. Construction and Assessment of Classification Rules. John Wiley & Sons, Chichester, 1997.

J. Hernández-Orallo, P. Flach, and C. Ferri. Brier Curves: A New Cost-Based Visualisation of Classifier Performance. In Proceedings of the 28th International Conference on Machine Learning (ICML 2011), pages 585–592. International Machine Learning Society, 2011.

J. Hernández-Orallo, P. Flach, and C. Ferri. A unified view of performance metrics: Translating threshold choice into expected classification loss. Journal of Machine Learning Research, 13:2813–2869, 2012.

H. Holzmann and M. Eulert. The role of the information set for forecasting – with applications to risk management. The Annals of Applied Statistics, 8(1):595–621, 2014. doi: 10.1214/13-AOAS709. URL https://doi.org/10.1214/13-AOAS709.

O. Koyejo, N. Natarajan, P. Ravikumar, and I.S. Dhillon. Consistent Binary Classification with Generalized Performance Metrics. In Z. Ghahramani, M. Welling, C. Cortes, N.D. Lawrence, and K.Q. Weinberger, editors, Advances in Neural Information Processing Systems 27, pages 2744–2752. Curran Associates, Inc., 2014.

F. Krüger and J.F. Ziegel. Generic Conditions for Forecast Dominance. Journal of Business & Economic Statistics, 39(4):972–983, 2021.

M. Kull and P.A. Flach. Reliability Maps: A Tool to Enhance Probability Estimates and Improve Classification Accuracy. In T. Calders, F. Esposito, E. Hüllermeier, and R. Meo, editors, Machine Learning and Knowledge Discovery in Databases. European Conference, ECML PKDD 2014, Nancy, France, September 15-19, 2014. Proceedings, Part II, pages 18–33. Springer Berlin Heidelberg, 2014.

M. Kull, T.M. Silva Filho, and P. Flach. Beyond sigmoid: How to obtain well-calibrated probabilities from binary classifiers with beta calibration. Electron. J. Statist., 11(2):5052–5080, 2017. doi: 10.1214/17-EJS1338SI.

J. Langford and B. Zadrozny. Estimating Class Membership Probabilities using Classifier Learners. In R. Cowell and Z. Ghahramani, editors, AISTATS 2005 – Proceedings of the Tenth International Workshop on Artificial Intelligence and Statistics, pages 198–205. The Society for Artificial Intelligence and Statistics, 2005.

C. Marrocco, R.P.W. Duin, and F. Tortorella. Maximizing the area under the ROC curve by pairwise feature combination. Pattern Recognition, 41(6):1961–1974, 2008.

A.K. Menon and R.C. Williamson. Bipartite Ranking: a Risk-Theoretic Perspective. The Journal of Machine Learning Research, 17(1):6766–6867, 2016.

A.K. Menon, X. Jiang, S. Vembu, C. Elkan, and L. Ohno-Machado. Predicting accurate probabilities with a ranking loss. In Proceedings of the 29th International Conference on Machine Learning, Edinburgh, Scotland, UK, pages 703–710, 2012.

A.H. Murphy and R.L. Winkler. Reliability of Subjective Probability Forecasts of Precipitation and Temperature. Journal of the Royal Statistical Society: Series C (Applied Statistics), 26(1):41–47, 1977. URL https://rss.onlinelibrary.wiley.com/doi/abs/10.2307/2346886.

J.C. Platt. Probabilities for SV Machines. In P.J. Bartlett, B. Schölkopf, D. Schuurmans, and A.J. Smola, editors, Advances in Large-Margin Classifiers, pages 61–74. MIT Press Cambridge, 2000.

22
M. Reid and R.C. Williamson. Information, Divergence and Risk for Binary Experiments. *Journal of Machine Learning Research*, 12:731–817, 2011.

R. Roelofs, N. Cain, J. Shlens, and M.C. Mozer. Mitigating bias in calibration error estimation. arXiv preprint arXiv:2012.08668, 2020.

M. Saerens, P. Latinne, and C. Decaestecker. Adjusting the Outputs of a Classifier to New a Priori Probabilities: A Simple Procedure. *Neural Computation*, 14(1):21–41, 2001.

M.J. Schervish. A general method for comparing probability assessors. *The Annals of Statistics*, 17(4):1856–1879, 1989.

C. Scott. A Generalized Neyman-Pearson Criterion for Optimal Domain Adaptation. In *Proceedings of Machine Learning Research, 30th International Conference on Algorithmic Learning Theory*, volume 98, pages 1–24, 2019.

V. Strassen. The Existence of Probability Measures with Given Marginals. *The Annals of Mathematical Statistics*, 36(2):423–439, 1965.

D. Tasche. A plug–in approach to maximising precision at the top and recall at the top. arXiv preprint arXiv:1804.03077, 2018.

H.L. Van Trees. *Detection, Estimation, and Modulation Theory, Part I*. John Wiley & Sons, 1968.

B. Zadrozny and C. Elkan. Obtaining Calibrated Probability Estimates from Decision Trees and Naive Bayesian Classifiers. In *Proceedings of the Eighteenth International Conference on Machine Learning*, ICML ’01, pages 609–616, 2001.

B. Zadrozny and C. Elkan. Transforming Classifier Scores into Accurate Multiclass Probability Estimates. In *Proceedings of the Eighth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD ’02, pages 694–699, New York, NY, USA, 2002. Association for Computing Machinery. URL https://doi.org/10.1145/775047.775151.

M.-J. Zhao, N. Edakunni, A. Pocock, and G. Brown. Beyond Fano’s Inequality: Bounds on the Optimal F-Score, BER, and Cost-Sensitive Risk and Their Implications. *The Journal of Machine Learning Research*, 14(1):1033–1090, 2013.

A. Proofs

A.1. Proof of Theorem 4.2

For the readers’ convenience, we present here an expanded version of the proof by Langford and Zadrozny (2005). This version, in particular, makes the informal part of the original proof between Eq. (2) and the following inequality more precise.

The first equation in (16b) is obtained through a combination of Proposition 2.4 and Proposition 4.1. For all $H \in \mathcal{H}$ and $t \in (0, 1)$, it can easily be shown that

$$L(H, t) = (1 - t) P[A] + \int_{H} (t - \Psi) dP.$$

Define the symmetric difference $M \triangle N$ of two sets $M$ and $N$ as

$$M \triangle N = M \setminus N \cup N \setminus M.$$

Then, since $L_{H}^{*}(t) = L(\{\Psi > t\}, t)$ by Theorem 32.4 of Devroye et al. (1996), it follows for all $t \in (0, 1)$ that

$$L(H(t), t) - L_{H}^{*}(t) = \int_{H(t) \triangle \{\Psi > t\}} |\Psi - t| dP.$$
Hence, by Fubini’s theorem it follows that
\[
\int_0^1 L(H(t), t) - L_{N}^*(t) \, dt = \int_0^1 \int_{\{(t, \omega) : h(t, \omega) = 1, \Psi(\omega) \leq t\}} (t - \Psi(\omega)) \, P(d\omega) \, dt \\
+ \int_0^1 \int_{\{(t, \omega) : h(t, \omega) = 0, \Psi(\omega) > t\}} (\Psi(\omega) - t) \, P(d\omega) \, dt
\]
\[
= \int \left( \int_0^1 1_{\{(t, \omega) : h(t, \omega) = 1, \Psi(\omega) \leq t\}} (t - \Psi(\omega)) \, dt \right) P(d\omega) \\
+ \int \left( \int_0^1 1_{\{(t, \omega) : h(t, \omega) = 0, \Psi(\omega) > t\}} (\Psi(\omega) - t) \, dt \right) P(d\omega).
\]

Define
\[
g(t, \omega) = \begin{cases} 
1, & \text{if } Z(\omega) > t, \\
0, & \text{if } Z(\omega) \leq t.
\end{cases}
\]

With this notation, it follows that \( \{Z > t\} = \{\omega : g(t, \omega) = 1\} \) and therefore
\[
\int_0^1 L(\{Z > t\}, t) - L_{N}^*(t) \, dt = \int \left( \int_0^1 1_{\{g(t, \omega) = 1, \Psi(\omega) \leq t\}} (t - \Psi(\omega)) \, dt \right) P(d\omega) \\
+ \int \left( \int_0^1 1_{\{g(t, \omega) = 0, \Psi(\omega) > t\}} (\Psi(\omega) - t) \, dt \right) P(d\omega).
\]

Hence, \((16b)\) is implied if we can show that for all \( \omega \in \Omega \)
\[
\int_0^1 1_{\{(t, \omega) : h(t, \omega) = 1, \Psi(\omega) \leq t\}} (t - \Psi(\omega)) \, dt + \int_0^1 1_{\{(t, \omega) : h(t, \omega) = 0, \Psi(\omega) > t\}} (\Psi(\omega) - t) \, dt
\]
\[
\geq \int_0^1 1_{\{(t, \omega) : g(t, \omega) = 1, \Psi(\omega) \leq t\}} (t - \Psi(\omega)) \, dt + \int_0^1 1_{\{(t, \omega) : g(t, \omega) = 0, \Psi(\omega) > t\}} (\Psi(\omega) - t) \, dt. \quad (27)
\]

Let \( I = \{t : g(t, \omega) = 0, h(t, \omega) = 1\} \) and \( J = \{t : g(t, \omega) = 1, h(t, \omega) = 0\} \). The definition of \( g \) implies
\[
\int_0^1 g(t, \omega) \, dt = Z(\omega) = \int_0^1 h(t, \omega) \, dt. \quad (28)
\]

Denoting by \( \ell(I) \) and \( \ell(J) \) the Lebesgue measures of \( I \) and \( J \) respectively, from \((28)\) follows
\[
\ell(I) = \ell(J).
\]

The definition of \( I \) and \( J \) moreover implies that \((27)\) is equivalent to
\[
\int_{\Psi(\omega)}^1 1_I(t) (t - \Psi(\omega)) \, dt + \int_0^{\Psi(\omega)} 1_J(t) (\Psi(\omega) - t) \, dt
\]
\[
\geq \int_{\Psi(\omega)}^1 1_J(t) (t - \Psi(\omega)) \, dt + \int_0^{\Psi(\omega)} 1_I(t) (\Psi(\omega) - t) \, dt. \quad (29)
\]

Consider now the case \( \Psi(\omega) < Z(\omega) \). Then
\[
[Z(\omega), 1] = [Z(\omega), 1] \cap [\Psi(\omega), 1] = \{t : g(t, \omega) = 0\} \cap [\Psi(\omega), 1],
\]
\[
[\Psi(\omega), Z(\omega)] = [0, Z(\omega)] \cap [\Psi(\omega), 1] = \{t : g(t, \omega) = 1\} \cap [\Psi(\omega), 1]
\]
and \( \emptyset = [Z(\omega), 1] \cap [0, \Psi(\omega)] = \{t : g(t, \omega) = 0\} \cap [0, \Psi(\omega)] \).
Making use of these observations and of $I \subset \{ t : g(t, \omega) = 0 \}$ and $J \subset \{ t : g(t, \omega) = 1 \}$, we obtain for the terms in (29)

\[
\int_{\Psi(\omega)}^{1} 1_{I}(t) (t - \Psi(\omega)) \, dt \geq (Z(\omega) - \Psi(\omega)) \ell(I),
\]

\[
\int_{0}^{\Psi(\omega)} 1_{J}(t) (\Psi(\omega) - t) \, dt \geq 0
\]

\[
\int_{\Psi(\omega)}^{1} 1_{J}(t) (t - \Psi(\omega)) \, dt \leq (Z(\omega) - \Psi(\omega)) \ell(J),
\]

\[
\int_{0}^{\Psi(\omega)} 1_{J}(t) (\Psi(\omega) - t) \, dt = 0.
\]

Since $\ell(I) = \ell(J)$ it follows that (29) and therefore also (27) are true in the case $\Psi(\omega) < Z(\omega)$. Assume now $\Psi(\omega) \geq Z(\omega)$. Then

\[
[0, Z(\omega)) = [0, Z(\omega)) \cap [0, \Psi(\omega)) = \{ t : g(t, \omega) = 1 \} \cap [0, \Psi(\omega)),
\]

\[
\emptyset = [0, Z(\omega)) \cap [\Psi(\omega), 1] = \{ t : g(t, \omega) = 1 \} \cap [\Psi(\omega), 1]
\]

and $[Z(\omega), \Psi(\omega)] = [Z(\omega), 1] \cap [0, \Psi(\omega)) = \{ t : g(t, \omega) = 0 \} \cap [0, \Psi(\omega))$.

Making use of these further observations and of $I \subset \{ t : g(t, \omega) = 0 \}$ and $J \subset \{ t : g(t, \omega) = 1 \}$, we obtain in this case for the terms in (29)

\[
\int_{\Psi(\omega)}^{1} 1_{I}(t) (t - \Psi(\omega)) \, dt \geq 0,
\]

\[
\int_{0}^{\Psi(\omega)} 1_{I}(t) (\Psi(\omega) - t) \, dt \geq (\Psi(\omega) - Z(\omega)) \ell(I)
\]

\[
\int_{\Psi(\omega)}^{1} 1_{J}(t) (t - \Psi(\omega)) \, dt = 0,
\]

\[
\int_{0}^{\Psi(\omega)} 1_{J}(t) (\Psi(\omega) - t) \, dt \leq (\Psi(\omega) - Z(\omega)) \ell(I).
\]

Since $\ell(I) = \ell(J)$ it again follows that (29) and therefore also (27) are true in the case $\Psi(\omega) \geq Z(\omega)$. This completes the proof.

\[\square\]

**A.2. Proof of Proposition 5.2**

Observe that for fixed $t \in [0, 1]$ and all $x \in [0, 1]$, it holds that

\[
\min(t, 1 - t) x (1 - x) \leq \min((1 - t) x, t (1 - x)) \leq x (1 - x).
\]

\[\text{(30a)}\]

From the properties of conditional probabilities, it follows that

\[
B(t) = E[\min((1 - t) \Psi, t (1 - \Psi))].
\]

\[\text{(30b)}\]

(30a) and (30b) together imply items 1, 2 and 3.

**Item 4.** For $0 \leq t \leq 1$, observe that

\[
B(t) = (1 - t) E[\Psi 1_{\{\Psi \leq t\}}] + t E[(1 - \Psi) 1_{\{\Psi > t\}}]
\]

\[
= E[\min(t, \Psi)] - t P[A].
\]
As a consequence of concavity, for each $t \in (0, 1]$ the left derivative $\frac{\partial^-}{\partial t} B(t)$ and for each $t \in [0, 1)$ the right derivative $\frac{\partial^+}{\partial t} B(t)$ of $B$ in $t$ exist and are finite. For fixed $\omega \in \Omega$, it holds that

$$\frac{\partial^-}{\partial t} \min(t, \Psi(\omega)) = 1_{\{t < \Psi\}}(\omega),$$

$$\frac{\partial^+}{\partial t} \min(t, \Psi(\omega)) = 1_{\{t \leq \Psi\}}(\omega).$$

By the dominated convergence theorem, this implies item 4.

**Item 5.** Because $B$ is concave, continuous and non-negative on $[0, 1]$ we know that it has a single maximum that is assumed by at least one $t^* \in (0, 1)$. All such $t^*$ must satisfy

$$\frac{d^-}{dt} B(t^*) \geq 0 \geq \frac{d^+}{dt} B(t^*) \iff 1 - P[A] - P[\Psi < t^*] \geq 0 \geq 1 - P[A] - P[\Psi \leq t^*]$$

$$\iff P[\Psi < t^*] \leq 1 - P[A] \leq P[\Psi \leq t^*].$$

Hence the $(1 - P[A])$-quantiles of $\Psi$ are the maximisers of $B$. This proves item 5.

**Item 6.** By Eq. (2.4) of Saerens et al. (2001), $\Psi_Q$ and $\Psi_P$ are related by

$$\Psi_Q = \frac{\frac{2}{p} \Psi_P}{\Psi_P + \frac{2}{1-p} (1 - \Psi_P)}.$$ 

This implies

$$\Psi_P \leq s \iff \Psi_Q \leq t,$$

and hence

$$P[\Psi_P \leq s \mid A] = Q[\Psi_Q \leq t \mid A] \quad \text{and} \quad P[\Psi_P > s \mid A^c] = Q[\Psi_Q > t \mid A^c].$$

Furthermore, by definition of $s$, it holds that

$$s \frac{(1-h)}{(1-s)p} = t \frac{(1-g)}{(1-t)q}.$$ 

This completes the proof of (22b). \qed

**A.3. Proof of Proposition 5.5**

From Proposition 5.2 it follows

$$\begin{align*}
(1 - q) P[A \cap \{ \Psi \leq q \}] + q P[A^c \cap \{ \Psi > q \}] &= L(\{ \Psi > q \}, q) \leq E[\Psi (1 - \Psi)]. \quad (31)
\end{align*}$$

By assumption, we have $P[\Psi > q] = P[A]$ which implies that

$$\begin{align*}
(1 - q) P[A \cap \{ \Psi \leq q \}] + q P[A^c \cap \{ \Psi > q \}] &= (1 - q) E[\Psi 1_{\{\Psi \leq q\}}] + q E[(1 - \Psi) 1_{\{\Psi > q\}}]
\end{align*}$$

$$\begin{align*}
&= E[\Psi 1_{\{\Psi \leq q\}}] - q E[\Psi 1_{\{\Psi \leq q\}}] + q P[A] - q E[\Psi 1_{\{\Psi > q\}}]
\end{align*}$$

$$\begin{align*}
&= E[\Psi 1_{\{\Psi \leq q\}}] + q (P[A] - E[\Psi])
\end{align*}$$

$$\begin{align*}
&= E[\Psi 1_{\{\Psi \leq q\}}]
\end{align*}$$

$$\begin{align*}
&= P[A] - P[A \cap \{ \Psi > q \}].
\end{align*}$$

Combining this with (31), we obtain

$$\begin{align*}
P[A] - P[A \cap \{ \Psi > q \}] \leq E[\Psi (1 - \Psi)]
\end{align*}$$

$$\iff P[A](1 - P[A]) - \text{cov}[1_A, 1_{\{\Psi > q\}}] \leq E[\Psi (1 - \Psi)].$$

26
Dividing both sides of this last inequality by \( P[A](1 - P[A]) \) gives the left-hand side of (26). Regarding the right-hand side of (26), observe that because of the \( \mathcal{H} \)-measurability of \( \Psi \) it holds that

\[
E[(1_A - \Psi)^2] = \min_{\text{\( \mathcal{H} \)-measurable}} E[(1_A - Z)^2] \\
\leq \min_{a,b \in \mathbb{R}} E[(1_A - (a 1_{\{\Psi > q\}} + b))^2].
\]

(32)

In plain language, the minimum squares error for approximating \( 1_A \) by general regression is lower than minimum squares error for approximating \( 1_A \) by linear regression on \( 1_{\{\Psi > q\}} \). It is well known (or follows from a short calculation) that the minimising linear regression coefficient \( a \) is given by

\[
a = \frac{\text{cov}[1_A, 1_{\{\Psi > q\}}]}{\text{var}[1_{\{\Psi > q\}}]} = \text{corr}[1_A, 1_{\{\Psi > q\}}].
\]

The optimising \( b \) is obtained as

\[
b = P[A] (1 - \text{corr}[1_A, 1_{\{\Psi > q\}}]).
\]

In addition, it holds for these numbers \( a \) and \( b \) that

\[
E[(1_A - (a 1_{\{\Psi > q\}} + b))^2] = \text{var}[1_A] - \text{var}[a 1_{\{\Psi > q\}} + b] \\
= P[A](1 - P[A]) - \text{corr}[1_A, 1_{\{\Psi > q\}}]^2 \text{var}[1_{\{\Psi > q\}}].
\]

Since \( E[(1_A - \Psi)^2] = E[\Psi (1 - \Psi)] \), the right-hand side inequality of (26) now follows from (32). \( \square \)