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Correspondence

A Distribution-Free Performance Bound in Error Estimation

LUC P. DEVROYE AND T. J. WAGNER, MEMBER, IEEE

***Abstract*—It is shown that distribution-free confidence intervals can be placed about the resubstitution estimate of the probability of error of any linear discrimination procedure.**

I. Introduction

In the discrimination problem the statistician is given an *observation* X, a random vector taking values in $\boldsymbol{R}^d$, and wishes to estimate its *state* $\theta \in \{1,2\}$. The only knowledge that the statistician has of the distribution of X, given $\theta = i$, is that which can be inferred from a sample of size n_i drawn from F_i where

$$P[X \le x \,|\, \theta = i] = F_i(x), \qquad i = 1,2. \tag{1}$$

The two samples, here called *data,* are denoted $X_1^1, \cdots, X_{n_1}^1$ and $X_1^2, \cdots, X_{n_2}^2$, respectively, and are assumed to be independent of X regardless of its state.

A discrimination procedure which has been frequently investigated in the past (see, for example, Duda and Hart [1, ch. 5]) is to estimate θ by $\hat{\theta}$ where

$$\hat{\theta} = \begin{cases} 1, & \text{if } w^t X \ge w_0 \\ 2, & \text{if } w^t X < w_0. \end{cases} \tag{2}$$

The vector $w^t = (w_1, \cdots, w_d)$ and the number w_0, called the weight vector and threshold weight, respectively, are chosen from the data. Regardless of what method is used to arrive at a weight vector and threshold weight, the statistician will always be interested in estimating

$$L_i = P[\hat{\theta} \ne i \,|X_1^1, \cdots, X^1{}_{n1}, X_1^2, \cdots, X_{n2}^2, \theta = i], \qquad i = 1,2,$$

a random variable whose value is just the frequency of errors when a large number of independent observations, all with state i, have their states estimated using (2).

The resubstitution estimates $\hat{L}_i$ of L_i are defined by

$$\hat{L}_2 = \frac{1}{n_2} \sum_1^{n_2} I_{[w^t X_j^2 \ge w_0]}$$

and

$$\hat{L}_1 = \frac{1}{n_1} \sum_1^{n_1} I_{[w^t X_j^1 < w_0]}.$$

These estimates have the appeal of being very simple to calculate once w and w_0 have been determined and, indeed, some procedures for finding w and w_0 involve the specific calculations above. For example, for a given $0 < \alpha < 1$, one may seek values w and w_0 such that, when $\hat{L}_1 \le \alpha$, $\hat{L}_2$ is minimized.

The question that we address ourselves to here is: how much confidence can the statistician place in these estimates, that is, for a given $\epsilon > 0$, what is

$$P[|\hat{L}_i - L_i| < \epsilon]. \tag{3}$$

There is, of course, no way of calculating (3) since the distribution functions (1) are unknown. However, if μ_i denotes the measure on the Borel sets corresponding to F_i and $\hat{\mu}_i$ denotes the empirical measure on the Borel sets for $X_1^i, \cdots, X_{n_i}^i$ (e.g., $\hat{\mu}_i(A)$ is the proportion of the X with state i falling in the set A), then

$$P[|L_i - \hat{L}_i| \ge \epsilon] \le P\left[\sup_{A \in \mathcal{C}_i} |\mu_i(A) - \hat{\mu}_i(A)| \ge \epsilon\right] \tag{4}$$

where $\mathcal{C}_i$ deontes the class of sets of the form $\{x : w^t x \ge w_0\}$, for $i = 2$, and $\{x : w^t x < w_0\}$, for $i = 1$. The random variable on the right in (4) is, in the one-dimensional case, essentially what is dealt with in the Glivenko–Cantelli theorem [2]. Indeed, for $d \ge 1$, Wolfowitz [2] showed that this random variable tends to zero with probability one as $n_i \to \infty$. While this gives the statistician some assurance that, for large n_i, his estimate of L_i will be close to the actual value uniformly in all procedures for determining w and w_0 (see Glick [3] for a thorough discussion of this point), he still falls short of getting a numerical grasp on (3).

Suppose now that $X_1, \cdots, X_n$ is a sample of size n drawn from the distribution function F. If μ denotes the measure corresponding to F and $\hat{\mu}$ denotes the empirical measure for $X_1, \cdots, X_n$, then Vapnik and Chervonenkis [4, theorem 2, p. 269] have shown that

$$P\left\{\sup_{A \in \mathcal{C}} |\mu(A) - \hat{\mu}(A)| \ge \epsilon\right\} \le 4s(\mathcal{C}, 2n)e^{-n\epsilon^2/8}$$

where $\mathcal{C}$ is a class of Borel sets in $\boldsymbol{R}^d$ and $S(\mathcal{C}, n)$ is the maximum over $x_1, \cdots, x_n$ of the number of sets in $\{\{x_1, \cdots, x_n\} \cap A : A \in \mathcal{C}\}$. For the class of "half planes" that we are considering here (e.g., $\mathcal{C}_1$ or $\mathcal{C}_2$),

$$s(\mathcal{C}_1, n) = \sum_0^d \binom{n}{k} \le n^d + 1, \qquad \text{if } n \ge d.$$

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The authors are with the Department of Electrical Engineering, University of Texas, Austin, TX 78712.

Applying these results to (4) yields

$$P[|\hat{L}_i - L_i| \geq \epsilon] \leq 4(1 + 2^d n_i^d)e^{-n_i\epsilon^2/8}, \qquad i = 1,2. \tag{5}$$

The significance of (5) is that the statistician knows that

$$P[|\hat{L}_i - L_i| < \epsilon] \geq 1 - 4(1 + 2^d n_i^d)e^{-n_i\epsilon^2/8}, \qquad i = 1,2$$

regardless of F_1,F_2. By constraining his decision procedure to be linear, he can get a distribution-free performance bound with the resubstitution estimates $\hat{L}_i$ independently of the procedure used to find w and w_0. This generalizes the result stated in [5] for $d = 1$ and left there as an open question for $d > 1$.

II. Extensions

This result has easy extensions. Suppose the statistician decides to use a rule of the form:

$$\hat{\theta} = \begin{cases} 1, & \text{if } w^t\Phi(X) \geq w_0 \\ 2, & \text{if } w^t\Phi(X) < w_0 \end{cases}$$

where

$$\Phi = \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_m \end{pmatrix}$$

is a fixed vector of real-valued measurable functions defined on $\boldsymbol{R}^d$ with $w^t = (w_1, \cdots ,w_m)$ and w_0 determined in some manner from the data. A distribution-free bound for

$$P[|\hat{L}_i - L_i| \geq \epsilon], \qquad i = 1,2,$$

can be obtained immediately by replacing X_j^i by $\Phi(X_j^i)$ so that m replaces d in (5). However, the Vapnik and Chervonenkis result allows a firmer bound if $s(\mathcal{C},n)$ can be computed, where $\mathcal{C}$ is the class of sets of the form $\{x \in \boldsymbol{R}^d : w^t\Phi(x) \geq w_0\}$ or $\{x \in \boldsymbol{R}^d : w^t\Phi(x) < w_0\}$. The early paper of Cover [6] contains some specific examples, including the important case where $w^t\Phi(x)$ is a polynomial of degree r in the components of x.

Suppose θ can now take values in $\{1, \cdots ,M\}$ where

$$P[X \leq x/\theta = i] = F_i(x), \qquad 1 \leq i \leq M.$$

The data become the sequence

$$X_1^1, \cdots ,X_{n1}^1, \cdots ,X_1^M, \cdots ,X_{nM}^M \tag{6}$$

where $X_1^i, \cdots ,X_{n_i}^i$ is a sample of size n_i drawn from F_i. The sequence (6) will be denoted simply by the vector D. The linear decision rule for M states is

$$\hat{\theta} = \text{smallest integer which achieves } \max_{1\leq i\leq M} \{w_i^tX + w_{i0}\}, \tag{7}$$

where, as before, the weights and thresholds $w_1,w_{10}, \cdots ,w_M,w_{M0}$ are determined in some manner from the data. If $L_i = P\{\hat{\theta} \neq i/D, \theta = i\}$, then its resubstitution estimate just counts the frequency of errors made by (7) on the sample $X_1^i, \cdots ,X_{n_i}^i$. It is not very difficult to see that a distribution-free bound for this case is given by

$$P[|L_i - \hat{L}_i| \geq \epsilon] \leq 4(1 + 2^d n_i^d)^{M-1}e^{-n_i\epsilon^2/8}, \quad 1 \leq i \leq M. \tag{8}$$

Finally, we may assume, in some situations, that θ is a random variable taking values in $\{1, \cdots ,M\}$ with an unknown distribution

$$P\{\theta = i\} = \pi_i, \qquad 1 \leq i \leq M. \tag{9}$$

The data $(X_1,\theta_1), \cdots ,(X_n,\theta_n)$ is now a sample of size n drawn from the distribution of (X,θ) which is determined from (1) and (9) while the random variable

$$L = P[\hat{\theta} \neq \theta \mid (X_1,\theta_1), \cdots ,(X_n,\theta_n)] = \sum_1^M \pi_i L_i$$

is the probability of error for (7) with the statistician's data and his method of choosing the weights and thresholds. The resubstitution estimate of L becomes

$$\hat{L} = \frac{1}{n}\sum_1^n I_{[\hat{\theta}_i \neq \theta_i]} = \sum_1^M \frac{N_i}{n}\hat{L}_i = \sum_1^M \hat{\pi}_i\hat{L}_i$$

where N_i is the number of observations in the data with state i and $\hat{\pi}_i$ is the usual frequency estimate of π_i, $1 \leq i \leq M$. $\hat{L}$ is, of course, the frequency of errors made on the data with (7). For, $0 < \alpha < 1$,

$$\begin{aligned} &P[|\hat{L} - L| \geq \epsilon] \\ &\quad\leq P\left[\sup_i |\hat{\pi}_i - \pi_i| \geq \alpha\epsilon/M\right] \\ &\quad+ P\left[\sup_i |\hat{\pi}_i - \pi_i| < \alpha\epsilon/M \text{ and } |\hat{L} - L| \geq \epsilon\right]. \end{aligned}$$

The second term above equals

$$\begin{aligned} &P\left[\sup_i |\hat{\pi}_i - \pi_i| < \alpha\epsilon/M \text{ and } \left|\sum_1^M \pi_i(\hat{L}_i - L_i)\right| \geq (1 - \alpha)\epsilon\right] \\ &\quad\leq \sum_1^M P[|\hat{\pi}_i - \pi_i| \leq \alpha\epsilon/M \text{ and } |\hat{L}_i - L_i| \geq (1 - \alpha)\epsilon/M\pi_i]. \end{aligned}$$

Since $(1 - \alpha)\epsilon/M\pi_i \geq 1$ will yield a probability of zero in each term above, we consider only terms with

$$\pi_i \geq (1 - \alpha)\epsilon/M.$$

Then

$$[|\hat{\pi}_i - \pi_i| \leq \alpha\epsilon/M] \subseteq [N_i \geq n\epsilon(1 - 2\alpha)/M]$$

and, from (5) and assuming $1 - 2\alpha > 0$,

$$\begin{aligned} &P[|\hat{\pi}_i - \pi_i| \leq \alpha\epsilon/M \text{ and } |\hat{L}_i - L_i| \geq (1 - \alpha)\epsilon/M\pi_i] \\ &\qquad\leq 4(1 + 2^d(n\epsilon(1 - 2\alpha)/M)^d)^{M-1}e^{-n\epsilon^3(1-\alpha)^2(1-2\alpha)/8M^3} \end{aligned}$$

Using Hoeffding's inequality [7], we see that, for $0 < \alpha < 1/2$,

$$\begin{aligned} &P[|L - \hat{L}| \geq \epsilon] \leq 2Me^{-2n\alpha^2\epsilon^2/M^2} \\ &\quad+ 4M(1 + 2^d(n\epsilon(1 - 2\alpha)/M)^d)^{M-1}e^{-n\epsilon^3(1-\alpha)^2(1-2\alpha)/8M^3}. \end{aligned} \tag{10}$$

No attempt here has been made to find the tightest bound possible. The interest in (10), as stressed earlier, is that it works for *all* $\pi_1, \cdots ,\pi_M, F_1, \cdots ,F_M$ and *all* ways of choosing the weights and thresholds.

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