

functions," *IEEE Trans. Inform. Theory*, vol. IT-15, pp. 525-531, 1969.

- [12] A. Crolotte and J. Pearl, "Asymptotic rate-distortion functions for coding precedence relations," *IEEE Trans. Inform. Theory*, vol.

IT-25, no. 1, pp. 80-82, Jan. 1979.

- [13] A. Crolotte, "Memory versus error tradeoffs in question-answering systems," Ph.D. dissertation, Univ. California, Los Angeles, UCLA-ENG-7753, July 1977.

# Distribution-Free Inequalities for the Deleted and Holdout Error Estimates

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**Abstract**—In the discrimination problem the random variable  $\theta$ , known to take values in  $\{1, \dots, M\}$ , is estimated from the random vector  $X$  taking values in  $\mathbb{R}^d$ . All that is known about the joint distribution of  $(X, \theta)$  is that which can be inferred from a sample  $(X_1, \theta_1), \dots, (X_n, \theta_n)$  of size  $n$  drawn from that distribution. A discrimination rule is any procedure which determines a decision  $\hat{\theta}$  for  $\theta$  from  $X$  and  $(X_1, \theta_1), \dots, (X_n, \theta_n)$ . The rule is called  $k$ -local if the decision  $\hat{\theta}$  depends only on  $X$  and the pairs  $(X_i, \theta_i)$ , for which  $X_i$  is one of the  $k$  closest to  $X$  from  $X_1, \dots, X_n$ . If  $L_n$  denotes the probability of error for a  $k$ -local rule given the sample, then estimates  $\hat{L}_n$  of  $L_n$  are determined for which  $P\{|\hat{L}_n - L_n| > \epsilon\} < A \exp(-Bn)$ , where  $A$  and  $B$  are positive constants depending only on  $d, M$ , and  $\epsilon$ .

## I. INTRODUCTION

IN THE discrimination problem a statistician makes an observation  $X$ , a random vector with values in  $\mathbb{R}^d$ , and wishes to estimate its state  $\theta$ , a random variable known to take values in  $\{1, \dots, M\}$ . All that he knows about the distribution of  $(X, \theta)$  is that which can be inferred from a sample  $(X_1, \theta_1), \dots, (X_n, \theta_n)$  of size  $n$  drawn from that distribution. The sample, commonly called *data*, is assumed to be independent of  $(X, \theta)$ . Using  $X$  and the data, the statistician makes a decision  $\hat{\theta}$  for  $\theta$  where his rule is any procedure which determines  $\hat{\theta}$  from  $X$  and the data.

The rules which we are interested in are called  $k$ -local rules. Here the estimate  $\hat{\theta}$  is a function of  $X$ , the  $k$  nearest observations to  $X$  from  $X_1, \dots, X_n$ , and the states of these  $k$  nearest observations. Because there may be ties in determining the  $k$  nearest observations to  $X$ , we use an independent sequence of random variables  $Z, Z_1, Z_2, \dots$

which itself is an independent identically distributed (i.i.d.) sequence with a uniform distribution on  $[0, 1]$ . Then  $X_i$  is nearer than  $X_j$  to  $X$  if

- a)  $\|X - X_i\| < \|X - X_j\|$ , or
- b)  $\|X - X_i\| = \|X - X_j\|$  and  $|Z - Z_i| < |Z - Z_j|$ , or
- c)  $\|X - X_i\| = \|X - X_j\|$ ,  $|Z - Z_i| = |Z - Z_j|$ , and  $i < j$ .

The event c) has probability zero and can be ignored. We will think of  $Z$  as being attached to  $X$  and of  $Z_i$  as being attached to  $X_i$  for  $i = 1, \dots, n$ . If a new independent observation  $X'$  is to have its state estimated, another random variable  $Z'$  is generated, but  $Z_1, \dots, Z_n$  remain the same. If  $(X^i, \theta^i, Z^i)$  denotes the  $i$ th-nearest observation, its state, and its attached random variable, respectively, then a  $k$ -local rule is any rule for which

$$\hat{\theta} = g(X, Z, (X^1, \theta^1, Z^1), \dots, (X^k, \theta^k, Z^k))$$

for some measurable function  $g$ .

The most familiar example of a  $k$ -local rule is the  $k$ -nearest neighbor rule [1], in which  $\hat{\theta}$  is taken to be the state which occurs most often among the  $k$  nearest observations to  $X$ . In the event that several states tie in this respect,  $\hat{\theta}$  is taken to be the state from those tied with the nearest observation to  $X$ .

For a  $k$ -local rule and the given data, the probability of error is

$$L_n = P\{\hat{\theta} \neq \theta | V_n\}$$

where

$$V_n = ((X_1, \theta_1, Z_1), \dots, (X_n, \theta_n, Z_n)).$$

The value taken by the random variable  $L_n$  is just the limiting frequency of errors made when a large number of independent observations have their states estimated with the given rule and data. Since  $L_n$  measures the effectiveness of the rule, and since it cannot be computed, the immediate need of the statistician is to estimate it as accurately as possible. Suppose, for example,  $n$  additional observations and their states  $(X_{n+1}, \theta_{n+1}), \dots,$

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$(X_{n+m}, \theta_{n+m})$  are available. One then could estimate  $L_n$  by the empirical frequency count

$$\hat{L}_n = \frac{1}{m} \sum_{i=1}^m I_{\{\hat{\theta}_{n+i} \neq \theta_{n+i}\}}$$

where  $\hat{\theta}_{n+i}$  is the estimate of  $\theta_{n+i}$  from  $X_{n+i}, Z_{n+i}$ , and  $V_n$  and where  $I_{\{\cdot\}}$  denotes the indicator function of the event  $\{\cdot\}$ . This estimate will be close to  $L_n$  if  $m$  is large, and since, conditioned on the data, the sequence  $I_{\{\hat{\theta}_{n+1} \neq \theta_{n+1}\}}, \dots, I_{\{\hat{\theta}_{n+m} \neq \theta_{n+m}\}}$  is a sequence of Bernoulli trials with expectation  $L_n$ , we have, using Hoeffding's inequality [2],

$$P\{|L_n - \hat{L}_n| \geq \epsilon | V_n\} \leq 2e^{-2m\epsilon^2}. \quad (1)$$

Inequality (1) is interesting because it does not depend on the data or a specific knowledge of the distribution of  $(X, \theta)$  and, at the same time, is reasonably tight. The difficulty with this estimate is that one rarely has  $m$  additional observations and states, and even if they were available, they would be included in the data. One wants then an estimate  $\tilde{L}_n$  of  $L_n$  which depends only on the data and for which  $P\{|\tilde{L}_n - L_n| \geq \epsilon\}$  can be upper-bounded by an expression which depends only on known quantities (e.g.,  $n, d, M, \epsilon$ ) and tends to zero with  $n$  as fast as possible. In short, one wants an estimate  $\tilde{L}_n$  which yields a good distribution-free upper bound for  $P\{|\tilde{L}_n - L_n| \geq \epsilon\}$ . We note here that since  $L_n$  and  $\tilde{L}_n$  are both functions of the data it is no longer possible to find such bounds for  $P\{|\tilde{L}_n - L_n| \geq \epsilon | V_n\}$ .

If  $\hat{\theta}(V_n, X, Z)$  denotes the function which first finds the  $k$  nearest points to  $X, Z$  from  $V_n$  and then uses  $g$  to get the value of  $\hat{\theta}$ , we can write the *resubstitution estimate*  $L_n^R$ , the *deleted estimate*  $L_n^D$ , and the *holdout estimate*  $L_n^H$  as

$$L_n^R = \frac{1}{n} \sum_{i=1}^n I[\hat{\theta}(V_n, X_i, Z_i) \neq \theta_i],$$

$$L_n^D = \frac{1}{n} \sum_{i=1}^n I[\hat{\theta}(V_{n,i}, X_i, Z_i) \neq \theta_i],$$

and

$$L_n^H = \frac{1}{s} \sum_{i=1}^s I[\hat{\theta}(V_n'', X_i, Z_i) \neq \theta_i],$$

respectively, where  $V_{n,i}$  denotes the sequence  $V_n$  with  $(X_i, \theta_i, Z_i)$  deleted and where  $V_n'' = (X_{s+1}, \theta_{s+1}, Z_{s+1}), \dots, (X_n, \theta_n, Z_n)$ , for  $n > s \geq 1$ . Notice that we must have  $n \geq k+1$  for  $L_n^D$  to be defined and  $n \geq k+s$  for  $L_n^H$  to be defined.

The main objective of this paper is to present distribution-free bounds for  $P\{|\hat{L}_n - L_n| \geq \epsilon\}$  when the rule used is a  $k$ -local rule and  $\hat{L}_n$  is one of the above estimates. The first distribution-free bound for  $k$ -local rules was found by Rogers and Wagner [3], who showed that

$$E(L_n^D - L_n)^2 \leq ((0.25 + 6k)/n) + (4k/n^2)$$

(see also [4], where the bound  $(1 + 6k)/n$  is obtained) so that

$$P\{|L_n^D - L_n| \geq \epsilon\} \leq ((0.25 + 6k)/n\epsilon^2) + (4k/n^2\epsilon^2)$$

by Chebyshev's inequality. The bounds derived in this paper, by contrast, will be exponential in  $n$  with an exponent depending on  $d, k$ , and  $\epsilon$ . Similar bounds will be derived for  $L_n^H$ . The resubstitution estimate has been shown to have exponential distribution-free bounds for linear discrimination rules [5]–[7], which are not local, and has been discounted for local rules because, when the distribution of  $X$  given  $\theta$  is absolutely continuous,  $L_n^R = 0$  with probability one for the single-nearest rule regardless of the value of  $L_n$ . In spite of this, we show that  $L_n^R$  is close to  $L_n^D$  and to  $L_n$  for large  $k$ .

## II. RESULTS

The bounds below use the constant  $\gamma_d$ , the maximum number of distinct points in  $\mathbb{R}^d$  which can share the same nearest neighbor. While one can easily see that  $\gamma_1 = 2$  and  $\gamma_2 = 6$ , no explicit formula for  $\gamma_d$  is known. It can be shown that  $\gamma_d \leq 3^d - 1$  for all  $d$  while other upper and lower bounds for  $d \geq 9$  are given in [8].

To economize on the use of parentheses in the formulas that follow,  $(abc)/(def)$  will be written  $abc/def$  (e.g., in an expression involving only multiplications and one division, the multiplications are done first).

*Theorem 1:* For  $k$ -local rules with  $k \leq n-1$ ,

$$P\{|L_n^D - L_n| \geq \epsilon\} \leq 2e^{-n\epsilon^2/18} + 6e^{-n\epsilon^3/108k(2+\gamma_d)}. \quad (2)$$

*Theorem 2:* For  $k$ -local rules with  $k \leq n-s$ ,

$$E(L_n - L_n^H)^2 \leq (1/2s) + (2sk/n) \quad (3)$$

and

$$P\{|L_n - L_n^H| \geq \epsilon\} \leq 2e^{-s\epsilon^2/2} + (2sk/n\epsilon). \quad (4)$$

By using an argument similar to the one used for Theorem 1, an exponential bound for  $L_n^H$  can be obtained which depends on  $d$ .

*Theorem 3:* For  $k$ -local rules with  $k \leq n-s$  and  $s < n\epsilon/12k(\gamma_d + 2)$ ,

$$P\{|L_n^H - L_n| \geq \epsilon\} \leq 2e^{-2s\epsilon^2/9} + 4e^{-n\epsilon^3/216k(\gamma_d + 2)}. \quad (5)$$

The holdout estimate always poses the problem of the selection of  $s$ . From Theorem 2 one might be tempted to conclude that  $s = \sqrt{n/4k}$  would be a good choice since it minimizes the bound (3) for  $E(L_n^H - L_n)^2$ . However, such a choice will not yield an exponential bound in (5). If one lets  $s = \rho n/k$ , for some  $0 < \rho < \epsilon/12(\gamma_d + 2) < 1$ , then the bound (5) is exponential in  $n$ . This is somewhat surprising since  $E(L_n^H - L_n)^2$  can go to zero at an algebraically slow rate in this case (see [3]). One might still wonder, however, if the dependence on  $d$  is necessary. The following example shows that it is.

*Example:* Put  $M = 2$ , and consider the nearest neighbor rule with  $n$  fixed and  $d = 2n$ . In  $\mathbb{R}^{2n}$  let the distribution of  $(X, \theta)$  put weight  $1/n$  at  $((0, \dots, 0), 1)$  and weight  $(1/2n) \cdot (1 - 1/n)$  at each of the points  $(e_i, 2)$ ,  $1 \leq i \leq 2n$ , where  $e_i$  is the  $i$ th unit vector in  $\mathbb{R}^{2n}$ . If  $A$  is the event that exactly one of the  $(X_i, \theta_i)$  equals  $((0, \dots, 0), 1)$  for  $1 \leq i \leq s$  and

none of the  $(X_i, \theta_i)$  do for  $s+1 \leq i \leq n$ , then, on  $A$ ,

$$L_n^H = \frac{1}{s}$$

and

$$L_n \geq \frac{1}{2n} \left(1 - \frac{1}{n}\right) (1+n) = \frac{1}{2} - \frac{1}{2n^2}$$

so that

$$L_n - L_n^H \geq \frac{1}{2} - \frac{1}{2n^2} - \frac{1}{s}.$$

Thus, whenever  $1/2 - 1/2n^2 - 1/s \geq \epsilon$ ,

$$P\{|L_n - L_n^H| \geq \epsilon\} \geq P\{A\} = \frac{s}{n} \left(1 - \frac{1}{n}\right)^{n-1} \geq \frac{s}{en} \quad (6)$$

since  $\exp((x-1)/x) \leq x$ ,  $0 \leq x \leq 1$ , implies  $(1-1/n)^{n-1} \geq e^{-1}$ . Thus if one picks  $s = \rho n$  for some  $\rho = \rho(\epsilon)$ , where  $0 < \rho < 1$ , then (6) shows that  $P\{|L_n - L_n^H| \geq \epsilon\}$  cannot go to zero exponentially fast in  $n$  uniformly in  $d$  and the distribution of  $(X, \theta)$ . In fact, when  $s = \rho n$ , (6) shows that it cannot even go to zero in  $n$  uniformly in  $d$  and the distribution of  $(X, \theta)$ .

We do not know if the dependence on  $d$  in (2) is necessary for the deleted estimate to have a distribution-free exponential bound.

If one considers the specific case of the  $k$ -nearest neighbor rule, then the above bounds can be improved somewhat by replacing  $k/n$  with  $\sqrt{k}/n$ . In both Theorem 4 and Theorem 5 below, one should be cautioned that  $k$  is fixed and not a function of  $n$ .

**Theorem 4:** For the  $k$ -nearest neighbor rule with  $M=2$  and  $k \leq n-1$ ,

$$E(L_n^D - L_n)^2 \leq (1/n) + (24\sqrt{k}/\sqrt{2\pi}n). \quad (7)$$

If  $M=2$  and  $k \leq n-s$ , then

$$E(L_n^H - L_n)^2 \leq (1/2s) + (8s\sqrt{k}/\sqrt{2\pi}n) \quad (8)$$

and

$$P\{|L_n^H - L_n| \geq \epsilon\} \leq 2e^{-s\epsilon^2/2} + (8s\sqrt{k}/\sqrt{2\pi}n\epsilon). \quad (9)$$

In fact, by using a large  $k$ , the resubstitution estimate becomes a reasonable estimate of  $L_n$ .

**Theorem 5:** For the  $k$ -nearest neighbor rule with  $M=2$  and  $k \leq n-1$ ,

$$E(L_n^R - L_n)^2 \leq 2E(L_n^D - L_n)^2 + 8/\sqrt{2\pi k}. \quad (10)$$

### III. PROOFS

If  $x_1, \dots, x_n$  is a sequence of distinct points in  $\mathbb{R}^d$  and if the nearest point or neighbor to  $x_j$  is found from  $x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n$  for  $1 \leq j \leq n$ , then as noted earlier, no point can be the nearest neighbor to more than  $\gamma_d$  of the remaining points. If the points are now the values assumed by the observations  $X_1, \dots, X_n$ , we can no longer make this statement because the distribution of  $X$  may have atoms so that  $X_1, \dots, X_n$  are not necessarily distinct.

Nevertheless, if we use the sequence  $Z_1, \dots, Z_n$  and the notion of "nearest" in Section I, we have the following easy lemma.

**Lemma 1:** Suppose  $(X_1, Z_1), \dots, (X_n, Z_n)$  is the sequence obtained from the data by omitting the states of each observation. If, for each  $j$ , the nearest neighbor to  $(X_j, Z_j)$  is found from  $(X_1, Z_1), \dots, (X_{j-1}, Z_{j-1}), (X_{j+1}, Z_{j+1}), \dots, (X_n, Z_n)$ , then no point  $(X_i, Z_i)$  can be the nearest neighbor to more than  $\gamma_d + 2$  of the remaining points.

**Lemma 2:** Suppose the probability distribution of the binary-valued sequence  $Y_1, \dots, Y_n$  is the same as that of  $Y_{\sigma(1)}, \dots, Y_{\sigma(n)}$  for every permutation  $\sigma$  of  $1, \dots, n$ . Then

$$P\left\{\left|\frac{1}{l} \sum_{i=1}^l Y_i - \frac{1}{n} \sum_{i=1}^n Y_i\right| \geq \epsilon\right\} \leq 2e^{-2l\epsilon^2}, \quad 1 \leq l \leq n.$$

**Proof:** If  $Q(y_1, \dots, y_n)$  is the probability distribution of  $Y_1, \dots, Y_n$ , then

$$Q(y_{\sigma(1)}, \dots, y_{\sigma(n)}) = Q(y_1, \dots, y_n)$$

for all  $\sigma$ , and

$$\begin{aligned} & P\left\{\left|\frac{1}{l} \sum_{i=1}^l Y_i - \frac{1}{n} \sum_{i=1}^n Y_i\right| \geq \epsilon\right\} \\ &= \frac{1}{n!} \sum_{\sigma} P\left\{\left|\frac{1}{l} \sum_{i=1}^l Y_{\sigma(i)} - \frac{1}{n} \sum_{i=1}^n Y_i\right| \geq \epsilon\right\} \\ &= \frac{1}{n!} \sum_{\sigma} \sum_{y_1, \dots, y_n} I_{\{|(1/l)\sum_{i=1}^l y_{\sigma(i)} - (1/n)\sum_{i=1}^n y_i| \geq \epsilon\}} \\ &\quad \cdot Q(y_1, \dots, y_n) \\ &= \sum_{y_1, \dots, y_n} Q(y_1, \dots, y_n) \\ &\quad \cdot \left(\frac{1}{n!} \sum_{\sigma} I_{\{|(1/l)\sum_{i=1}^l y_{\sigma(i)} - (1/n)\sum_{i=1}^n y_i| \geq \epsilon\}}\right) \\ &\leq \sum_{y_1, \dots, y_n} Q(y_1, \dots, y_n) 2e^{-2l\epsilon^2} = 2e^{-2l\epsilon^2} \end{aligned}$$

where the inequality follows from Hoeffding [2, sec. 6, theorem 4].

**Proof of Theorem 1:** We consider one-local rules first. Suppose

$$(X, \theta, Z), (X_1, \theta_1, Z_1), \dots, (X_{n+m}, \theta_{n+m}, Z_{n+m})$$

are i.i.d. with

$$V_n = (X_1, \theta_1, Z_1), \dots, (X_n, \theta_n, Z_n)$$

$$U_n = (X_{n+1}, \theta_{n+1}, Z_{n+1}), \dots, (X_{n+m}, \theta_{n+m}, Z_{n+m})$$

$$T_n = (X_1, \theta_1, Z_1), \dots, (X_{n+m}, \theta_{n+m}, Z_{n+m}).$$

We shall write  $V_{n,i}$ ,  $U_{n,i}$ ,  $T_{n,i}$  to denote the corresponding sequences with  $(X_i, \theta_i, Z_i)$  deleted. As before,  $V_n$  denotes the data used with  $X, Z$  to estimate  $\theta$ . The sequence  $U_n$  and its concatenation with  $V_n$ , denoted by  $T_n$ , are used

only in the proof. Let

$$\begin{aligned} L_n &= P\{\hat{\theta}(V_n, X, Z) \neq \theta | V_n\} \\ L_{n1} &= \frac{1}{m} \sum_{i=1}^m I\{\hat{\theta}(V_n, X_{n+i}, Z_{n+i}) \neq \theta_{n+i}\} \\ L_{n2} &= \frac{1}{m} \sum_{i=1}^m I\{\hat{\theta}(T_{n,n+i}, X_{n+i}, Z_{n+i}) \neq \theta_{n+i}\} \\ L_{n3} &= \frac{1}{n+m} \sum_{i=1}^{n+m} I\{\hat{\theta}(T_{n,i}, X_i, Z_i) \neq \theta_i\} \\ L_{n4} &= \frac{1}{n} \sum_{i=1}^n I\{\hat{\theta}(T_{n,i}, X_i, Z_i) \neq \theta_i\} \\ L_n^D &= \frac{1}{n} \sum_{i=1}^n I\{\hat{\theta}(V_n, X_i, Z_i) \neq \theta_i\}. \end{aligned}$$

Our proof consists of noting that

$$\begin{aligned} P\{|L_n - L_n^D| \geq \epsilon\} &\leq P\{|L_n - L_{n1}| \geq \epsilon/6\} \\ &\quad + P\{|L_{n1} - L_{n2}| \geq 2\epsilon/6\} \\ &\quad + P\{|L_{n2} - L_{n3}| \geq \epsilon/6\} \\ &\quad + P\{|L_{n3} - L_{n4}| \geq \epsilon/6\} \\ &\quad + P\{|L_{n4} - L_n^D| \geq \epsilon/6\} \quad (11) \end{aligned}$$

and showing that each term can be bounded in a distribution-free way by picking  $m$  properly.

1) Using Hoeffding's inequality for sums of independent  $[0, 1]$ -valued random variables [2], we have

$$P\{|L_n - L_{n1}| \geq \epsilon\} \leq 2e^{-2m\epsilon^2}.$$

2) We have

$$\begin{aligned} P\{|L_{n1} - L_{n2}| \geq \epsilon\} &\leq P\left\{\frac{1}{m} \sum_{i=1}^m I[\hat{\theta}(V_n, X_{n+i}, Z_{n+i}) \neq \hat{\theta}(T_{n,n+i}, X_{n+i}, Z_{n+i})] \geq \epsilon\right\} \\ &\leq P\left\{\frac{1}{m} \sum_{i=1}^m I_{A(n+i)} \geq \epsilon\right\} \end{aligned}$$

where, for  $l = 1, \dots, n+m$ ,  $A(l)$  is the event that  $(X_{n+j}, Z_{n+j})$  is the nearest neighbor to  $(X_l, Z_l)$  from  $T_{n,l}$  for some  $j = 1, \dots, m$ , excluding  $j = l - n$  if  $l > n$ . To use Lemma 2, we symmetrize the sequence  $I_{A(1)}, \dots, I_{A(n+m)}$  as follows. Let  $Y_1, \dots, Y_{n+m}$  be a random permutation of  $1, \dots, n+m$ . Then  $I_{A(Y_1)}, \dots, I_{A(Y_{n+m})}$  satisfies the conditions of Lemma 2, and

$$\begin{aligned} &P\left\{\frac{1}{m} \sum_{i=1}^m I_{A(n+i)} \geq \epsilon\right\} \\ &\leq P\left\{\frac{1}{m} \sum_{i=1}^m I_{A(Y_i)} \geq \epsilon\right\} \\ &= P\left\{\frac{1}{m} \sum_{i=1}^m I_{A(Y_i)} - \frac{1}{n+m} \sum_{i=1}^{n+m} I_{A(i)} \geq \epsilon - \frac{1}{n+m} \sum_{i=1}^{n+m} I_{A(i)}\right\} \\ &\leq 2e^{-2m(\epsilon/2)^2} \end{aligned}$$

whenever

$$\frac{1}{n+m} \sum_{i=1}^{n+m} I_{A(i)} \leq \epsilon/2. \quad (12)$$

However, since each  $(X_{n+j}, Z_{n+j})$  can be the nearest neighbor of at most  $(\gamma_d + 2)$  other points from  $T_n$ , we see that  $\sum_{i=1}^{n+m} I_{A(i)} \leq (\gamma_d + 2)m$ , and thus (12) is valid whenever  $(\gamma_d + 2)m < (n+m)\epsilon/2$ .

3) Lemma 2 can be applied immediately to  $L_{n2} - L_{n3}$  and  $L_{n3} - L_{n4}$  to yield

$$P\{|L_{n2} - L_{n3}| \geq \epsilon\} \leq 2e^{-2m\epsilon^2}$$

$$P\{|L_{n3} - L_{n4}| \geq \epsilon\} \leq 2e^{-2n\epsilon^2}.$$

4) Finally,

$$\begin{aligned} &P\{|L_{n4} - L_n^D| \geq \epsilon\} \\ &\leq P\left\{\frac{1}{n} \sum_{i=1}^n I[\hat{\theta}(T_{n,i}, X_i, Z_i) \neq \hat{\theta}(V_n, X_i, Z_i)] \geq \epsilon\right\} \\ &\leq P\left\{\frac{1}{n} \sum_{i=1}^n I_{A(i)} \geq \epsilon\right\} \\ &= 0, \quad \text{if } m(\gamma_d + 2) < n\epsilon. \end{aligned}$$

Taking  $m = n\epsilon/6(\gamma_d + 2)$  and using inequality (11), we see that

$$P\{|L_n - L_n^D| \geq \epsilon\} \leq 2e^{-n\epsilon^2/18} + 6e^{-m\epsilon^2/18}$$

which yields (2). For an arbitrary  $k$ , it suffices to replace  $(\gamma_d + 2)$  by  $k\gamma_d + 2 \leq k(\gamma_d + 2)$  since no  $(X_i, Z_i)$  can be one of the  $k$  nearest neighbors to more than  $k\gamma_d + 2$  of the points in  $V_{n,i}$ .

*Proof of Theorem 2:* Letting

$$V'_n = (X_1, \theta_1, Z_1), \dots, (X_s, \theta_s, Z_s)$$

and

$$V''_n = (X_{s+1}, \theta_{s+1}, Z_{s+1}), \dots, (X_n, \theta_n, Z_n),$$

we have

$$\begin{aligned} |L_n - L_n^H| &\leq |L_n - E(L_n^H | V''_n)| + |E(L_n^H | V''_n) - L_n^H| \\ &\leq P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V''_n, X, Z) | V_n\} \\ &\quad + |E(L_n^H | V''_n) - L_n^H| \end{aligned}$$

since

$$\begin{aligned} E(L_n^H | V''_n) &= P\{\hat{\theta}(V''_n, X, Z) \neq \theta | V''_n\} \\ &= P\{\hat{\theta}(V''_n, X, Z) \neq \theta | V_n\} \end{aligned}$$

and

$$\begin{aligned} &|P\{\hat{\theta}(V_n, X, Z) \neq \theta | V_n\} - P\{\hat{\theta}(V''_n, X, Z) \neq \theta | V_n\}| \\ &\leq P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V''_n, X, Z) | V_n\}. \end{aligned}$$

Using  $|a+b|^r \leq 2^{r-1}(|a|^r + |b|^r)$  for  $r \geq 1$ , we have

$$\begin{aligned} E(L_n - L_n^H)^2 &\leq 2P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z)\} \\ &\quad + 2E(L_n^H - E(L_n^H | V_n''))^2 \\ &\leq 2P\left\{\bigcup_{i=1}^s \{(X_i, Z_i) \text{ is among the } k \right. \\ &\quad \left. \text{nearest to } (X, Z)\}\right\} \\ &\quad + 2\frac{1}{4s} \\ &\leq \frac{2sk}{n} + \frac{1}{2s} \end{aligned} \quad (13)$$

which proves (3). Also,

$$\begin{aligned} P\{|L_n - L_n^H| \geq \epsilon\} &\leq P\{|L_n^H - E(L_n^H | V_n'')| \geq \epsilon/2\} \\ &\quad + P\{P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z) | V_n\} \geq \epsilon/2\} \\ &\leq E\{P\{|L_n^H - E(L_n^H | V_n'')| \geq \epsilon/2 | V_n''\}\} \\ &\quad + \frac{2}{\epsilon} P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z)\} \\ &\leq 2e^{-2s(\epsilon/2)^2} + 2sk/n\epsilon \end{aligned}$$

using Hoeffding's inequality and Markov's inequality. This proves Theorem 2.

*Proof of Theorem 3:* Using the notation of the proofs of Theorems 1 and 2, consider  $k$  equal to one. From the argument of Theorem 2 we have

$$\begin{aligned} P\{|L_n - L_n^H| \geq \epsilon\} &\leq 2e^{-2s\epsilon^2/9} \\ &\quad + P\{P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z) | V_n\} \geq 2\epsilon/3\}. \end{aligned}$$

Letting

$$L_n^* = \frac{1}{m} \sum_{i=1}^m I[\hat{\theta}(V_n, X_{n+i}, Z_{n+i}) \neq \hat{\theta}(V_n'', X_{n+i}, Z_{n+i})]$$

we have

$$\begin{aligned} P\{P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z) | V_n\} \geq 2\epsilon/3\} &\leq P\{|L_n^* - P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z) | V_n\}| \geq \epsilon/3\} \\ &\quad + P\{L_n^* \geq \epsilon/3\} \\ &\leq 2e^{-2m\epsilon^2/9} + P\{L_n^* \geq \epsilon/3\} \end{aligned}$$

where, for the first term, we first condition the probability on  $V_n$  and use Hoeffding's inequality. Also,

$$P\{L_n^* \geq \epsilon/3\} \leq P\left\{\frac{1}{m} \sum_{i=1}^m I_{C(n+i)} \geq \epsilon/3\right\}$$

where  $C(n+j)$  is the event that the closest point to  $(X_{n+j}, Z_{n+j})$  from  $V_n$  is  $(X_i, Z_i)$  for some  $1 \leq i \leq s$ . However, if  $D(j)$  is the event that the closest point to  $(X_j, Z_j)$  from  $T_{n,j}$  is  $(X_i, Z_i)$  for some  $1 \leq i \leq s$  or  $n < i \leq n+m$ , then

$$C(n+j) \subseteq D(n+j)$$

and

$$\begin{aligned} P\{L_n^* \geq \epsilon/3\} &\leq P\left\{\frac{1}{m} \sum_{i=1}^m I_{D(n+i)} \geq \epsilon/3\right\} \\ &\leq P\left\{\frac{1}{m} \sum_{i=1}^m I_{D(Y_i)} \geq \epsilon/3\right\} \end{aligned}$$

where  $Y_1, \dots, Y_{n+m}$  is an independent random permutation of  $1, \dots, n+m$ . Using the same arguments as Theorem 1, we see that this last term is bounded by  $2e^{-2m(\epsilon/6)^2}$  if  $1/(n+m)\sum_{i=1}^{n+m} I_{D(i)} \leq \epsilon/6$ . This occurs if  $(\gamma_d+2)(s+m) < (\epsilon/6)(n+m)$ . Taking  $m = n\epsilon/12(\gamma_d+2)$  and  $s < n\epsilon/12(\gamma_d+2)$  yields the theorem for  $k=1$  after collecting terms. For arbitrary  $k$ , we need only replace  $(\gamma_d+2)$  by  $k(\gamma_d+2)$ .

*Lemma 3:* If  $P\{Y=j\} = \binom{n}{j}(1/2)^n$ ,  $0 \leq j \leq n$ , then

$$P\{|Y - n/2| \leq a/2\} < 4a/\sqrt{2\pi n}$$

for all positive integers  $a$ .

*Proof:* We make repeated use of Feller's [9] approximation for  $n!$ . If  $n$  is even, the maximal term of the binomial expansion is

$$\frac{1}{2^n} \binom{n}{n/2} \leq \frac{2}{\sqrt{2\pi n}} \exp\left(\frac{1}{12n} - \frac{2}{6n+1}\right) < \frac{2}{\sqrt{2\pi n}}.$$

Hence  $P\{|Y - n/2| \leq a/2\}$  is upper-bounded by

$$(a+1)2/\sqrt{2\pi n} < 4a/\sqrt{2\pi n}.$$

For  $n$  odd,  $n \geq 3$ , the maximal term is

$$\begin{aligned} \frac{1}{2^n} \binom{n}{(n-1)/2} &< \frac{1}{2^{n-1}} \binom{n-1}{(n-1)/2} \\ &< \frac{1}{\sqrt{2\pi(n-1)}} < \frac{2}{\sqrt{\pi n}}. \end{aligned}$$

Thus

$$P\{|Y - n/2| \leq a/2\} \leq 2a/\sqrt{\pi n} < 4a/\sqrt{2\pi n}.$$

*Lemma 4:* For  $k$ -local estimates with  $k \leq n-1$ ,

$$\begin{aligned} E(L_n - L_n^D)^2 &\leq 1/n + 6P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_{n,1}, X, Z)\} \\ &\leq 1/n + 6k/n. \end{aligned}$$

Lemma 4 is proved in [4]. It can, in implicit form, also be found in [3].

*Proof of Theorem 4:* We will show that

$$P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z)\} \leq 4s\sqrt{k}/\sqrt{2\pi} n. \quad (14)$$

A combination of (14) and (13) yields (8); (7) follows from Lemma 4 and (14) upon noting that  $V_n'' = V_{n,1}$  if  $s=1$ .

Let  $N$ ,  $N_1$ , and  $N_2$  be the number of  $(X_i, Z_i)$  that are among the  $k$  nearest neighbors to  $(X, Z)$  and for which, respectively,  $1 \leq i \leq s$ ,  $\theta_i = 1$ , and  $\theta_i = 2$ . Conditioned on  $(X^{k+1}, Z^{k+1}, X, Z)$ , the random variables  $N$  and  $|N_1 - N_2|$

are independent. Thus

$$\begin{aligned} & P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z)\} \\ & \leq \sum_{j=1}^s P\{N=j, |N_1 - N_2| \leq j\} \\ & = E\left\{\sum_{j=1}^s P\{N=j|X, Z\} \right. \\ & \quad \left. \cdot P\{|N_1 - N_2| \leq j|X, Z, X^{k+1}, Z^{k+1}\}\right\}. \end{aligned}$$

If  $\binom{k}{j} = 0$  for  $j > k$ ,

$$P\{N=j|X, Z\} = \frac{\binom{k}{j}\binom{n-k}{s-j}}{\binom{n}{s}}.$$

Also, by Lemma 3,

$$\begin{aligned} & P\{|N_1 - N_2| \leq j|X, Z, X^{k+1}, Z^{k+1}\} \\ & = P\{|N_1 - k/2| \leq j/2|X, Z, X^{k+1}, Z^{k+1}\} \\ & \leq 4j/\sqrt{2\pi k}. \end{aligned}$$

Collecting bounds and using a property of the hypergeometric distribution [10] yields

$$\begin{aligned} P\{\hat{\theta}(V_n, X, Z) \neq \hat{\theta}(V_n'', X, Z)\} & \leq \sum_{j=1}^s j \frac{\binom{k}{j}\binom{n-k}{s-j}}{\binom{n}{s}} \frac{4}{\sqrt{2\pi k}} \\ & = 4ks/n\sqrt{2\pi k} \\ & = 4s\sqrt{k}/\sqrt{2\pi} n. \end{aligned}$$

*Proof of Theorem 5:* From  $(a+b)^2 \leq 2(a^2+b^2)$  and

$$|L_n - L_n^R| \leq |L_n - L_n^D| + \left| \frac{1}{n} \sum_{i=1}^n I\{\hat{\theta}(V_n, X_i, Z_i) \neq \hat{\theta}(V_n'', X_i, Z_i)\} \right|,$$

we deduce

$$\begin{aligned} E(L_n - L_n^R)^2 & \leq 2E(L_n - L_n^D)^2 \\ & \quad + 2E\left(\frac{1}{n} \sum_{i=1}^n I\{\hat{\theta}(V_n, X_i, Z_i) \neq \hat{\theta}(V_n'', X_i, Z_i)\}\right)^2 \\ & \leq 2E(L_n - L_n^D)^2 \\ & \quad + 2P\{\hat{\theta}(V_n, X_1, Z_1) \neq \hat{\theta}(V_n'', X_1, Z_1)\} \\ & \leq 2E(L_n - L_n^D)^2 \\ & \quad + 2 \sup_{x,z} P\{|N_1(x, z) - N_2(x, z)| \leq 1\} \\ & \leq 2E(L_n - L_n^D)^2 + 8/\sqrt{2\pi k} \end{aligned}$$

where we use Lemma 3 and where  $N_1(x, z)$  and  $N_2(x, z)$  are as in the proof of Theorem 4 after replacement of  $(X, Z)$  by  $(x, z)$ .

#### REFERENCES

- [1] T. M. Cover and P. E. Hart, "Nearest neighbor pattern classification," *IEEE Trans. Inform. Theory*, vol. IT-13, pp. 21–27, Jan. 1967.
- [2] W. Hoeffding, "Probability inequalities for sums of bounded random variables," *J. Amer. Stat. Ass.*, vol. 58, pp. 13–30, 1963.
- [3] W. H. Rogers and T. J. Wagner, "A finite sample distribution-free performance bound for local discrimination rules," *Ann. Stat.*, vol. 6, pp. 506–514, 1978.
- [4] L. P. Devroye and T. J. Wagner, "Nonparametric discrimination and density estimation," Information Systems Research Laboratory, Univ. Texas, Austin, Tech. Rep. 183, 1976.
- [5] V. N. Vapnik and A. Ya. Chervonenkis, "Theory of uniform convergence of frequencies of events to their probabilities and problems of search for an optimal solution from empirical data," *Automation and Remote Control*, vol. 32, pp. 207–217, 1971.
- [6] L. P. Devroye and T. J. Wagner, "A distribution-free performance bound in error estimation," *IEEE Trans. Inform. Theory*, vol. IT-22, pp. 586–587, Sept. 1976.
- [7] —, "Distribution-free performance bounds with the resubstitution error estimate," in *Proc. 1977 Computer Society Conf. Pattern Recognition and Image Processing*, Troy, NY, 1977, pp. 323–326.
- [8] C. Rogers, "Covering a sphere with spheres," *Mathematika*, vol. 10, pp. 157–164, 1963.
- [9] W. Feller, *An Introduction to Probability Theory and Its Applications*, vol. 1. New York: Wiley, 1968.
- [10] G. Roussas, *A First Course in Mathematical Statistics*. Reading, MA: Addison-Wesley, 1973.