

Recursive Feature Elimination by Sensitivity Testing

I. SUPPLEMENTARY MATERIAL

A. Generalization of Theorem 2.1

In this Section, we will prove a stronger version of Theorem 2.1, generalizing it to apply to a product distribution \mathcal{D} and to a function other than parity.

There are two parameters that are important in generalizing Theorem 2.1, ρ and I_{\min} . Under a uniform distribution, each feature j has equal probability of being either 1 or 0. Under a product distribution, one of these two probabilities may be larger than the other. We use $\rho > 0$ to denote the maximum, over all features j , of the ratio between the larger and the smaller of these two probabilities, for product distribution \mathcal{D} . Thus, for example, if each feature j is 1 with probability $3/4$ and 0 with probability $1/4$, then $\rho = 3$.

When the examples are labeled according to a parity function (on a subset of the variables), flipping the value of a relevant feature j in a random example drawn from \mathcal{D} always changes the value of the function. For other functions g , flipping the value of a relevant feature j in a random example drawn from \mathcal{D} will change the value of g with some non-zero probability. We denote the minimum of that probability, over all relevant j , by I_{\min} . This is the minimum *influence* of a relevant variable of g , with respect to distribution \mathcal{D} (cf. [1]).

For the uniform distribution with g being a parity function, $\rho = 1$ and $I_{\min} = 1$.

The generalized theorem replaces the polynomial dependence of m on $\frac{1}{\frac{1}{2} - \epsilon}$ in Theorem 2.1 with a polynomial dependence on $\frac{1}{\frac{1}{2}I_{\min} - \rho\epsilon}$.

Theorem I.1. *Suppose a machine learning algorithm is used to learn a classifier M for a Boolean target concept f defined on n Boolean features, where the target concept labels examples according to the value of a Boolean function g , computed on a fixed subset of the features. Suppose M has true error rate $\epsilon < \frac{1}{2}$, with respect to a product distribution \mathcal{D} , where $2\rho\epsilon \leq I_{\min}$. Then there is a quantity t that is polynomial in n , $\ln \frac{1}{\delta}$, and $\frac{1}{\frac{1}{2}I_{\min} - \rho\epsilon}$, with the following property: for all $0 < \delta < 1$, if the $\tilde{R}(j)$ values for all n features are computed using M and an i.i.d. sample of size t , drawn from distribution \mathcal{D} , then with probability least $1 - \delta$, the computed $\tilde{R}(j)$ values for all the relevant features will be higher than the computed $\tilde{R}(j)$ values for the irrelevant features.*

Proof. Consider a random example a drawn from \mathcal{D} . Flipping any relevant bit in a reverses the output of f with probability at least I_{\min} .

Let $P(a)$ denote the probability of drawing assignment a from distribution \mathcal{D} . By the definition of ρ , for any bit j ,

$\frac{1}{\rho}P(a) \leq P(a_{-j}) \leq \rho P(a)$. Here a_{-j} denotes the assignment produced by flipping bit j of a .

Let A denote the set of assignments in $\{0, 1\}^n$ such that $M(a) \neq f(a)$.

Consider a relevant variable j of f . First, we will lower bound the probability, for random a drawn from distribution \mathcal{D} , that $f(a) \neq M(a_{-j})$. It is easy to see that $f(a) \neq M(a_{-j})$ iff one of the following two conditions holds: (1) $f(a) \neq f(a_{-j})$, and $a_{-j} \notin A$, or (2) $f(a) = f(a_{-j})$, and $a_{-j} \in A$. Thus the probability that $f(a) \neq M(a_{-j})$ is lower bounded by the probability that Condition (1) holds. We will now lower bound that probability.

$$\begin{aligned} & \text{Prob}[f(a) \neq f(a_{-j}) \text{ and } a_{-j} \notin A] \\ & \geq \text{Prob}[f(a) \neq f(a_{-j})] - \text{Prob}[a_{-j} \in A] \\ & \geq I_{\min} - \rho\epsilon \end{aligned} \quad (1)$$

The last inequality above uses the fact that the total probability mass of A is ϵ , and therefore the total probability mass of assignments a such that $a_{-j} \in A$ is at most $\rho\epsilon$.

Thus, for relevant variable j , for random a drawn from \mathcal{D} , $\text{Prob}[f(a) \neq M(a_{-j})] \geq I_{\min} - \rho\epsilon$.

Now consider the case where j is an irrelevant variable. In this case, the only way that $f(a) \neq M(a_{-j})$ is if $a_{-j} \in A$, which happens with probability at most $\rho\epsilon$. Therefore, $\text{Prob}[f(a) \neq M(a_{-j})] \leq \rho\epsilon$.

In the statement of the theorem, we assumed that $I_{\min} > 2\rho\epsilon$. Let $\tau = \frac{1}{2}I_{\min} - \rho\epsilon$.

Now suppose we compute the $\tilde{R}(j)$ values for all features j using an i.i.d. random sample \mathcal{X} drawn from \mathcal{D} and labeled according to f . Let $t = \frac{1}{2\tau^2} \ln \frac{n}{\delta}$ be the size of this sample. Recall that $\tilde{R}(j)$ is the difference between the accuracy of M on \mathcal{X} , and the accuracy of M on the sample derived from \mathcal{X} by flipping j in each example. This second accuracy measures the percentage of examples a for which $f(a) = M(a_{-j})$. Let $d(j)$ be the percentage of examples a for which $f(a) \neq M(a_{-j})$. It follows that for any pair of features j' and j'' , $\tilde{R}(j') \geq \tilde{R}(j'')$ iff $d(j') \geq d(j'')$. We will prove the following claim: with probability at least $1 - \delta$, $d(j) > \frac{1}{2}I_{\min}$ for each relevant feature j , and $d(j) < \frac{1}{2}I_{\min}$ for each irrelevant feature j . This suffices to prove the theorem.

To prove the claim, consider a random a drawn from \mathcal{D} . We can view the test of whether $f(a) \neq M(a_{-j})$ as a Bernoulli trial, with success when the inequality holds. Thus if j is a relevant variable, the probability of success is at least $I_{\min} - \rho\epsilon$. If j is an irrelevant variable, the probability of success is at most $\rho\epsilon$.

With this view, we can apply a standard bound of Hoeffding. Consider a sequence of m independent Bernoulli trials, each

with probability p of success. Suppose that out of these m trials, the observed fraction of successes is \hat{p} . The bound of Hoeffding states that for any $c > 0$, $Prob[\hat{p} \geq p + c] \leq e^{-2mc^2}$ [2]. By exchanging the role of failures and successes, it immediately follows that the inequality $Prob[\hat{p} \leq p - c] \leq e^{-2mc^2}$ also holds. Thus if $m \geq \frac{1}{2c^2} \ln \frac{1}{\delta}$, we have the following two inequalities

$$Prob[\hat{p} \geq p + t] \leq \delta \quad (2)$$

$$Prob[\hat{p} \leq p - t] \leq \delta \quad (3)$$

We apply these two inequalities to the tests performed in computing $d(j)$ from \mathcal{X} . Consider a random assignment a drawn from \mathcal{D} . If j is relevant, then the probability of success (i.e., that $f(a) \neq M(a_{-j})$) is at least $(I_{min} - \rho\epsilon)$. If j is irrelevant, then the probability of success is at most $\rho\epsilon$. The assignments in \mathcal{X} correspond to $\frac{1}{2\tau^2} \ln \frac{n}{\delta}$ Bernoulli trials. Because $\tau = \frac{1}{2}I_{min} - \rho\epsilon$, applying the above bounds with $c = \tau$ and $s = \frac{1}{2\tau^2} \ln \frac{n}{\delta}$ implies that the following holds for each feature j : If j is relevant, then $Prob[d(j) \leq \frac{1}{2}I_{min}] \leq \frac{\delta}{n}$, and if j is irrelevant, then $Prob[d(j) \geq \frac{1}{2}I_{min}] \leq \frac{\delta}{n}$.

Since there are n features, it follows that with probability at least $1 - \delta$, the $d(j)$ values for the relevant variables will all be greater than $\frac{1}{2}I_{min}$, and the $d(j)$ values for the irrelevant features will be less than $\frac{1}{2}I_{min}$. \square

The condition $\epsilon < I_{min}/(2\rho)$ in the above theorem limits its applicability to arbitrary functions g , even under the uniform distribution. For example, consider the consensus function (which is correlation immune): $g(x_1, \dots, x_k) = 1$ iff $x_1 = x_2 = \dots = x_k$. Under the uniform distribution, the value of I_{min} for the consensus function is $1/2^{k-2}$. For $k = 4$, the condition $\epsilon < I_{min}/(2\rho)$ would then be satisfied only if the error ϵ of model M was less than $1/8$.

We note that while it might be possible to prove a version of the theorem with a somewhat less restrictive condition, there are inherent limits as to what can be proved. For example, suppose g is a function on k variables that classifies at least 75% of its 2^k possible examples as negative. (The consensus function on 3 variables has this property.) Then the model that predicts negative on all examples has exactly 75% accuracy. Using RFEST with such a model, there is no hope of distinguishing relevant from irrelevant variables.

REFERENCES

- [1] L. Hellerstein and R. A. Servedio, "On pac learning algorithms for rich boolean function classes," *Theoretical Computer Science*, vol. 384, no. 1, pp. 66 – 76, 2007, theory and Applications of Models of Computation.
- [2] W. Hoeffding, "Probability inequalities for sums of bounded random variables," *Journal of the American Statistical Association*, vol. 58, no. 301, pp. 13–30, 1963.