A SIMPLE MEASURE OF CONDITIONAL DEPENDENCE

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ABSTRACT. We propose a coefficient of conditional dependence between two random variables $Y$ and $Z$ given a set of other variables $X_1, \ldots, X_p$, based on an i.i.d. sample. The coefficient has a long list of desirable properties, the most important of which is that under absolutely no distributional assumptions, it converges to a limit in $[0, 1]$, where the limit is 0 if and only if $Y$ and $Z$ are conditionally independent given $X_1, \ldots, X_p$, and is 1 if and only if $Y$ is equal to a measurable function of $Z$ given $X_1, \ldots, X_p$. Using this statistic, we devise a new variable selection algorithm, called Feature Ordering by Conditional Independence (FOCI), which is model-free, has no tuning parameters, and is provably consistent under sparsity assumptions. A number of applications to synthetic and real datasets are worked out.

1. Introduction

The problem of measuring the amount of dependence between two random variables is an old problem in statistics. Numerous methods have been proposed over the years. For recent surveys, see [12, 33]. The literature on measures of conditional dependence, on the other hand, is not so large, especially in the non-parametric setting. This is the focus of this paper.

The non-parametric conditional independence testing problem can be relatively easily solved for discrete data using the classical Cochran–Mantel–Haenszel test [14, 37]. This test can be adapted for continuous random variables by binning the data [31] or using kernels [17, 27, 48, 52, 63].

Besides these, there are methods based on estimating conditional cumulative distribution functions [36, 41], conditional characteristic functions [53], conditional probability density functions [54], empirical likelihood [55], mutual information and entropy [32, 43, 46], copulas [1, 51, 58], distance correlation [23, 50, 60], and other approaches [47]. A number of interesting ideas based on resampling and permutation tests have been proposed in recent years [5, 10, 48].

The main contribution of this paper is a new coefficient of conditional dependence between two random variables $Y$ and $Z$ given a set of other variables $X_1, \ldots, X_p$, based on i.i.d. data. The coefficient is inspired by a
similar measure of univariate dependence recently proposed in [12]. The main features of our coefficient are the following:

1. it has a simple expression,
2. it is fully non-parametric,
3. it has no tuning parameters,
4. there is no need for estimating conditional densities, conditional characteristic functions, or mutual information,
5. it can be estimated from data very quickly, in time $O(n \log n)$ where $n$ is the sample size,
6. asymptotically, it converges to a limit in $[0,1]$, where the limit is 0 if and only if $Y$ and $Z$ are conditionally independent given $X_1,\ldots,X_p$, and is 1 if and only if $Y$ is equal to a measurable function of $Z$ given $X_1,\ldots,X_p$, and
7. all of the above hold under absolutely no assumptions on the laws of the random variables.

As an application of this measure of conditional dependence, we propose a new variable selection algorithm, called Feature Ordering by Conditional Independence (FOCI), which is model-free, has no tuning parameters, and is provably consistent under sparsity assumptions.

The paper is organized as follows. The definition and properties of our coefficient are presented in Section 2. This is followed by a result about hypothesis testing in Section 3. Our variable selection method is introduced in Section 4 and the theorem about its consistency is stated in Section 5. Applications to simulated and real data are presented in Section 6. The remaining sections are devoted to proofs.

2. The coefficient

Let $Y$ be a random variable and $\mathbf{X} = (X_1,\ldots,X_p)$ and $\mathbf{Z} = (Z_1,\ldots,Z_q)$ be random vectors, all defined on the same probability space. Here $q \geq 1$ and $p \geq 0$. The value $p = 0$ means that $\mathbf{X}$ has no components at all. Let $\mu$ be the law of $Y$. We propose the following quantity as a measure of the degree of conditional dependence of $Y$ and $\mathbf{Z}$ given $\mathbf{X}$:

$$T = T(Y,\mathbf{Z}|\mathbf{X}) := \frac{\int \mathbb{E}(\text{Var}(\mathbb{P}(Y \geq t|\mathbf{Z},\mathbf{X})|\mathbf{X}))d\mu(t)}{\int \mathbb{E}(\text{Var}(1_{\{Y \geq t\}}|\mathbf{X}))d\mu(t)}.$$  

(2.1)

In the denominator, $1_{\{Y \geq t\}}$ is the indicator of the event $\{Y \geq t\}$. If the denominator equals zero, $T$ is undefined. (We will see below that this happens if and only if $Y$ is almost surely equal to a measurable function of $\mathbf{X}$, which is a degenerate case that we will ignore.) If $p = 0$, then $\mathbf{X}$ has no components, and the conditional expectations and variances given $\mathbf{X}$ should be interpreted as unconditional expectations and variances. In this case we will write $T(Y,\mathbf{Z})$ instead of $T(Y,\mathbf{Z}|\mathbf{X})$.

Note that $T$ is a non-random quantity that depends only the joint law of $(Y,\mathbf{X},\mathbf{Z})$. Before stating our theorem about $T$, let us first see why $T$ is
a reasonable measure of conditional dependence. Since taking conditional expectation decreases variance, we have that for any $t$,

$$\text{Var}(1_{\{Y \geq t\}}|X) \geq \text{Var}(\mathbb{P}(Y \geq t|Z, X)|X).$$

This shows that the numerator in (2.1) is less than or equal to the denominator, and so $T$ is always between 0 and 1. Now, if $Y$ and $Z$ are conditionally independent given $X$, then $\mathbb{P}(Y \geq t|Z, X)$ is a function of $X$ only, and hence \(\text{Var}(\mathbb{P}(Y \geq t|Z, X)|X) = 0\). Therefore in this situation, $T = 0$. We will show later that the converse is also true. On the other hand, if $Y$ is almost surely equal to a measurable function of $Z$ given $X$, then $\mathbb{P}(Y \geq t|Z, X) = 1_{\{Y \geq t\}}$ for any $t$. Therefore in this case, $T = 1$. Again, we will prove later that the converse is also true. The following theorem summarizes these properties of $T$.

**Theorem 2.1.** Suppose that $Y$ is not almost surely equal to a measurable function of $X$ (when $p = 0$, this means that $Y$ is not almost surely a constant). Then $T$ is well-defined and $0 \leq T \leq 1$. Moreover, $T = 0$ if and only if $Y$ and $Z$ are conditionally independent given $X$, and $T = 1$ if and only if $Y$ is almost surely equal to a measurable function of $Z$ given $X$. When $p = 0$, conditional independence given $X$ simply means unconditional independence.

Having defined $T$, the main question is whether $T$ can be efficiently estimated from data. We will now present a consistent estimator of $T$, which is our conditional dependence coefficient. Our data consists of $n$ i.i.d. copies $(Y_1, X_1, Z_1), \ldots, (Y_n, X_n, Z_n)$ of the triple $(Y, X, Z)$, where $n \geq 2$. For each $i$, let $N(i)$ be the index $j$ such that $X_j$ is the nearest neighbor of $X_i$ with respect to the Euclidean metric on $\mathbb{R}^p$, where ties are broken uniformly at random. Let $M(i)$ be the index $j$ such that $(X_j, Z_j)$ is the nearest neighbor of $(X_i, Z_i)$ in $\mathbb{R}^{p+q}$, again with ties broken uniformly at random. Let $R_i$ be the rank of $Y_i$, that is, the number of $j$ such that $Y_j \leq Y_i$. If $p \geq 1$, our estimate of $T$ is

$$T_n = T_n(Y, Z|X) := \frac{\sum_{i=1}^{n}(\min\{R_i, R_{M(i)}\} - \min\{R_i, R_{N(i)}\})}{\sum_{i=1}^{n}(R_i - \min\{R_i, R_{N(i)}\})}.$$ 

If $p = 0$, let $L_i$ be the number of $j$ such that $Y_j \geq Y_i$, let $M(i)$ denote the $j$ such that $Z_j$ is the nearest neighbor of $Z_i$ (ties broken uniformly at random), and let

$$T_n = T_n(Y, Z) := \frac{\sum_{i=1}^{n}(\min\{R_i, R_{M(i)}\} - L_i^2)}{\sum_{i=1}^{n}L_i(n - L_i)}.$$ 

In both cases, $T_n$ is undefined if the denominator is zero. The following theorem proves that $T_n$ is indeed a consistent estimator of $T$.

**Theorem 2.2.** Suppose that $Y$ is not almost surely equal to a measurable function of $X$. Then as $n \to \infty$, $T_n \to T$ almost surely.
Remarks. (1) The statistic $T_n$ can be computed in $O(n \log n)$ time because nearest neighbors can be determined in $O(n \log n)$ time and ranks can also be calculated in $O(n \log n)$ time.

(2) No assumptions on the joint law of $(Y, X, Z)$ are needed other than the non-degeneracy condition that $Y$ is not almost surely equal to a measurable function of $X$. This condition is inevitable, because if this does not hold, then the question of conditional independence becomes ambiguous.

(3) Although the limit of $T_n$ is guaranteed to be in $[0, 1]$, the actual value of $T_n$ for finite $n$ may lie outside this interval.

(4) It is not easy to explain why $T_n$ is a consistent estimator of $T$ without going into the details of the proof, so we will not make that attempt here.

(5) We have not given a name to $T_n$, but if an acronym is desired for easy reference, one may call it CODEC, which is an acronym for Conditional Dependence Coefficient. In fact, this is the acronym that we use in the R code for computing $T_n$.

(6) An R package will soon be made available. For now, the code can be downloaded from https://statweb.stanford.edu/~souravc/foci.R

This R program contains the code for computing $T_n$ as well as the code for the variable selection algorithm FOCI presented in Section 4 below.

(7) Besides variable selection, another natural area of applications of our coefficient is graphical models. This is currently under investigation.

3. Testing conditional independence

The theorems of the previous section raise the possibility of constructing a consistent test for conditional independence based on $T_n$. However, it is known that this is an impossible task, even for a single alternative hypothesis, if we demand that the level of the test be asymptotically uniformly bounded by some given $\alpha$ over the whole null hypothesis space [49]. For the statistic $T_n$, the main problem is that although we know $T_n \to 0$ if and only if $Y$ and $Z$ are conditionally independent given $X$, the rate at which this convergence happens may depend on the joint law of $(Y, X, Z)$. In fact, we believe (without proof) that the convergence can be arbitrarily slow.

Still, it is possible to construct sequences of tests that achieve level 0 pointwise asymptotically [49] and are consistent against arbitrarily large classes of alternatives. Fix any $p, q \geq 1$. For each $n \geq 1$ and $\varepsilon \in (0, 1]$, let $\psi_{n,\varepsilon}$ be the test that rejects the hypothesis of conditional independence when $T_n(Y, Z|X) > \varepsilon$. Then the following result is an obvious corollary of Theorems 2.1 and 2.2.

**Theorem 3.1.** Fix $p, q \geq 1$ and $\varepsilon > 0$. Let $\mathcal{P}$ be the class of all joint laws of $(Y, X, Z)$ where $Y$ is a real-valued random variable, $X$ is a $p$-dimensional random vector, $Z$ is a $q$-dimensional random vector, $Y$ is not almost surely equal to a measurable function of $X$, and $Y$ and $Z$ are conditionally independent given $X$. Let $\psi_{n,\varepsilon}$ be defined as above. For $P \in \mathcal{P}$, let $\mathbb{P}_P$ denote
probabilities computed under $P$. Then for any $P \in \mathcal{P}$,
\[
\lim_{n \to \infty} P_P(\psi_n, \varepsilon \text{ rejects}) = 0.
\]
On the other hand, if $Q_\varepsilon$ denotes the set of all joint laws of $(Y, X, Z)$ such that $T(Y, Z|X) > \varepsilon$, then for any $Q \in Q_\varepsilon$,
\[
\lim_{n \to \infty} P_Q(\psi_n, \varepsilon \text{ rejects}) = 1.
\]
Finally, the set $Q_\varepsilon$ increases as $\varepsilon$ decreases, and if $Q$ is the set of all joint laws of $(Y, X, Z)$ such that $Y$ and $Z$ are not conditionally independent given $X$, then
\[
Q = \bigcup_{\varepsilon \in (0, 1]} Q_\varepsilon,
\]
showing that we can have consistent tests with pointwise asymptotic level 0 against arbitrarily large classes of alternatives.

In the absence of quantitative bounds, the above theorem is not useful from a practical point of view because it does not tell us how to choose $\varepsilon$ in a given problem. To obtain quantitative bounds, it is necessary to have more information about the joint law of $(Y, X, Z)$. Whether it will be possible to extract the required information from data is not clear. This is a future direction of research that is currently under investigation.

Incidentally, if we only want to test independence of $Y$ and $Z$, and not conditional independence given $X$, then it is easy to do it using $T_n(Y, Z)$ and a permutation test.

4. Feature Ordering by Conditional Independence (FOCI)

In this section we propose a new variable selection algorithm for multivariate regression using a forward stepwise algorithm based on our measure of conditional dependence. The commonly used variable selection methods in the statistics literature use linear or additive models. This is true of the classical methods [6, 13, 21, 25, 28, 29, 40, 57] as well as the more modern ones [11, 22, 44, 61, 65, 66]. These methods are powerful and widely used in practice. However, they sometimes run into problems when significant interaction effects or nonlinearities are present. We will later show an example where methods based on linear and additive models fail to select any of the relevant predictors, even in the complete absence of noise.

Such problems can sometimes be overcome by model-free methods [2, 3, 7–10, 24, 29, 30, 59]. These, too, are powerful and widely used techniques, and they perform better than model-based methods if interactions are present. On the flip side, their theoretical foundations are usually weaker than those of model-based methods.

The method that we are going to propose below, called Feature Ordering by Conditional Independence (FOCI), attempts to combine the best of both worlds by being fully model-free, as well as having a proof of consistency under a set of assumptions.
The method is as follows. First, choose $j_1$ to be the index $j$ that maximizes $T_n(Y, X_j)$. Having obtained $j_1, \ldots, j_k$, choose $j_{k+1}$ to be the index $j \not\in \{j_1, \ldots, j_k\}$ that maximizes $T_n(Y, X_j | X_{j_1}, \ldots, X_{j_k})$. Continue like this until arriving at the first $k$ such that $T_n(Y, X_{j_{k+1}} | X_{j_1}, \ldots, X_{j_k}) \leq 0$, and then declare the chosen subset to be $\hat{S} := \{j_1, \ldots, j_k\}$. If there is no such $k$, define $\hat{S}$ to be the whole set of variables. It may also happen that $T_n(Y, X_{j_1}) \leq 0$. In that case declare $\hat{S}$ to be empty.

Although it is not required theoretically, we recommend that the predictor variables be standardized before running the algorithm. We will see later that FOCI performs well in examples, even if the true dependence of $Y$ on $X$ is nonlinear in a complicated way. In the next section we prove the consistency of FOCI under a set of assumptions on the law of $(Y, X)$.

If computational time is not an issue, one can try to add $m \geq 2$ variables at each step instead of just one. Although we do not explore this idea in this paper, it is possible that this gives improved results in certain situations. Similarly, one can try a forward-backward version of FOCI, analogous to the forward-backward version of ordinary stepwise selection.

### 5. Consistency of FOCI

Let $(Y, X)$ be as in the previous section. For any subset of indices $S \subseteq \{1, \ldots, p\}$, let $X_S := (X_j)_{j \in S}$, and let $S^c := \{1, \ldots, p\} \setminus S$. In the machine learning literature, a subset $S$ is sometimes called sufficient \[59\] if $Y$ and $X_{S^c}$ are conditionally independent given $X_S$. This includes the possibility that $S$ is the empty set, when it simply means that $Y$ and $X$ are independent. Sufficient subsets are known as Markov blankets in the literature on graphical models [42, Section 3.2.1], and are closely related to the concept of sufficient dimension reduction in classical statistics [11, 15, 35]. If we can find a small subset of predictors that is sufficient, then our job is done, because these predictors contain all the relevant predictive information about $Y$ among the given set of predictors, and the statistician can then fit a predictive model based on this small subset of predictors.

For any subset $S$, let

$$Q(S) := \int \var \left( \mathbb{P}(Y \geq t | X_S) \right) d\mu(t),$$

where $\mu$ is the law of $Y$. We will prove later (Lemma [9,2]) that $Q(S') \geq Q(S)$ whenever $S' \supseteq S$, with equality if and only $Y$ and $X_{S^c \setminus S}$ are conditionally independent given $X_S$. Thus if $S' \supseteq S$, the difference $Q(S') - Q(S)$ is a measure of how much extra predictive power is added by appending $X_{S' \setminus S}$ to the set of predictors $X_S$.

Let $\delta$ be the smallest number such that for any insufficient subset $S$, there is some $j \not\in S$ such that $Q(S \cup \{j\}) \geq Q(S) + \delta$. In other words, if $S$ is insufficient, there exists some index $j \not\in S$ such that appending $X_j$ to $X_S$ increases the predictive power by at least $\delta$. The main result of this
section, stated below, says that if $\delta$ is not too close to zero, then under some regularity assumptions on the law of $(Y, X)$, the subset selected by FOCI is sufficient with high probability. Note that a sparsity assumption is hidden in the condition that $\delta$ is not very small, because the definition of $\delta$ ensures that there is at least one sufficient subset of size $\leq 1/\delta$.

To prove our result, we need the following two technical assumptions on the joint distribution of $(Y, X)$. It is possible that the assumptions can be relaxed.

(A1) There is a number $L$ such that for any $S$ of size $\leq 1/\delta$, any $x, x' \in \mathbb{R}^S$, and any $t \in \mathbb{R}$,
\[ |\mathbb{P}(Y \leq t | X_S = x) - \mathbb{P}(Y \leq t | X_S = x')| \leq L \|x - x'\| . \]

(A2) There is a number $B$ such that for any $S$ of size $\leq 1/\delta$, the support of $X_S$ has diameter $\leq B$.

Assumption (A1) says that a small change in a small set of predictors do not change the conditional law of $Y$ by much. This is certainly not an unreasonable assumption. Assumption (A2) looks more restrictive, but since we can freely apply transformations to the predictors before carrying out the analysis, we can always make them bounded.

The following theorem shows that under the above assumptions, the subset chosen by FOCI is sufficient with high probability.

**Theorem 5.1.** Suppose that $\delta > 0$, and that the assumptions (A1) and (A2) hold. Let $\hat{S}$ be the subset selected by FOCI with a sample of size $n$. There are positive real numbers $C_1$, $C_2$ and $C_3$ depending only on $L$, $B$ and $\delta$ such that $\mathbb{P}(\hat{S} \text{ is sufficient}) \geq 1 - C_1 p^{C_2} e^{-C_3 n}$.

The main implication of Theorem 5.1 is that if $\delta$ is not too close to zero, and $n \gg \log p$, then with high probability, FOCI chooses a sufficient set of predictors. In particular, this theorem allows $p$ to be quite large compared to $n$, as long as $\delta$ is not too small.

6. Examples

In this section we present some applications of our methods to simulated examples and real datasets. In all examples, the covariates were standardized prior to the analysis.

**Example 6.1** (Simulated example for CODEC). Let $X_1$ and $X_2$ be independent Uniform$[0, 1]$ random variables, and define
\[ Y := X_1 + X_2 \mod 1 . \]

The relationship between $Y$ and $(X_1, X_2)$ has three main features:

1. $Y$ is a function of $(X_1, X_2)$,
2. unconditionally, $Y$ is independent of $X_2$, and
3. conditional on $X_1$, $Y$ is a function of $X_2$. 
Simulations showed that all three features are effectively captured by our coefficient $T_n$. We took $n = 1000$, and computed $T_n(Y, (X_1, X_2))$, $T_n(Y, X_2)$, $T_n(Y, X_2|X_1)$ in 1000 independent simulations. About 95 percent of the time, $T_n(Y, (X_1, X_2))$ took values between 0.88 and 0.94, in agreement with the fact that $Y$ is a function of $(X_1, X_2)$. Similarly, 95 percent of time $T_n(Y, X_2|X_1)$ lay between 0.88 and 0.94, as we would expect from the fact that $Y$ is a function of $X_2$ conditional on $X_1$. On the other hand, the value of $T_n(Y, X_2)$ was between $-0.07$ and $0.07$ in 95 percent of the simulations, again in agreement with the fact that $Y$ and $X_2$ are unconditionally independent.

Existing methods from the literature are unable to capture the strong conditional dependency between $Y$ and $X_2$ given $X_1$. For example, in a typical simulation, the partial correlation between $Y$ and $X_2$ given $X_1$ turned out to be only $-0.001$, completely failing to detect that $Y$ is actually a function $X_2$ conditional on $X_1$. The recently proposed conditional distance correlation [60] also turned out to be quite small — approximately $0.092$ — which, while statistically significantly different than zero, is far from detecting that $Y$ is a function of $X_2$ given $X_1$.

**Example 6.2 (Simulated example for FOCI).** In this example we investigate the performance of FOCI in a simulated dataset and compare it to some popular methods of variable selection. We chose to have 1000 covariates $X_1, \ldots, X_{1000}$, which were generated as i.i.d. standard normal random variables. The response $Y$ was defined as the following noiseless function of the first three variables $X_1, X_2$ and $X_3$:

$$Y = X_1X_2 + \sin(X_1X_3).$$  \hfill (6.1)

There is nothing special about this particular function. It was chosen as an arbitrary example of a function with complicated nonlinearities and interactions. We also tried to avoid explicit monotone relationships between $Y$ and the $X_i$’s, because most methods are good at detecting monotone relationships.

With a sample of size 2000, we compared the performance of FOCI with the following popular algorithms for variable selection: Forward stepwise, Lasso [57], the Dantzig selector [11], and SCAD [22]. The tuning parameters for Lasso, Dantzig selector and SCAD were chosen using 10-fold cross-validation, and the AIC criterion was used for stopping in forward stepwise. Standard R packages were used for all computations. In this example we did not compare with methods that only give an ordering of variables or prediction rules (such as random forests [3]), or methods for which standard prescriptions for choosing tuning parameter values are not available (such as SPAM [44] or mutual information [3]).

Table 1 displays the results of our comparisons. The table shows that only FOCI was able to select the correct subset. Forward stepwise, Lasso and SCAD selected long lists of variables that did not include the relevant ones, while the Dantzig selector did not select any variables.
Table 1. Comparison table for Example 6.2 (simulated example with $p = 1000$ covariates, $Y = X_1X_2 + \sin(X_1X_3)$, and sample size $n = 2000$).

| Method            | Selected variables                                                                 |
|-------------------|-----------------------------------------------------------------------------------|
| FOCI              | 1, 2, 3.                                                                          |
| Forward stepwise  | 247 variables were selected, but 1, 2, and 3 were not in the list.                  |
| Lasso             | 28, 43, 68, 95, 96, 189, 241, 262, 275, 292, 351, 362, 387, 403, 490, 514, 526, 537, |
|                   | 560, 578, 583, 623, 635, 675, 787, 814, 834, 914, 965, 968.                         |
| Dantzig selector  | No variables were selected.                                                         |
| SCAD              | 28, 43, 68, 241, 262, 292, 351, 387, 403, 537, 583, 623, 675, 814, 834, 968.         |

Table 2. Number of variables selected using different methods and the corresponding mean squared prediction errors in Example 6.3 (spambase data).

| Method          | Subset size | MSPE  |
|-----------------|-------------|-------|
| FOCI            | 26          | 0.036 |
| Forward stepwise| 45          | 0.039 |
| Lasso           | 56          | 0.038 |
| Dantzig selector| 51          | 0.038 |
| SCAD            | 33          | 0.039 |

Example 6.3 (Spambase data). In this example we apply FOCI to a widely used benchmark dataset, known as the spambase data [18], and compare its performance with other methods.

We used the version of the dataset that is available at the UCI Machine Learning Repository. The data consists of 4601 observations, each corresponding to one email, and 57 features for each observation. The response variable is binary, indicating whether the email is a spam email or not.

We compared FOCI with forward stepwise, Lasso, Dantzig selector and SCAD, as in the previous example. As before, the tuning parameters for Lasso, Dantzig selector and SCAD were chosen using 10-fold cross-validation, and the AIC criterion was used for stopping in forward stepwise.

We chose 80% of the observations at random as the training set and kept the rest for testing. The variables were selected by running the competing algorithms on the training set. For each method, after selecting the variables, we fitted a predictive model using random forests. Random forests were used because they gave better prediction errors than any other technique (such as linear models).
Table 3. Number of variables selected using different methods and the corresponding mean squared prediction errors in Example 6.4 (Polish companies bankruptcy data).

| Method          | Subset size | MSPE  |
|-----------------|-------------|-------|
| FOCI            | 10          | 0.015 |
| Forward stepwise| 24          | 0.016 |
| Lasso           | 48          | 0.017 |
| Dantzig selector| 27          | 0.017 |
| SCAD            | 3           | 0.021 |

The mean squared prediction errors were then estimated using the test set. The results are shown in Table 2. From this table, we see that FOCI gave a slightly better prediction error than the other methods (0.036 for FOCI versus 0.038 or 0.039 for every other method), even though the size of the subset selected by FOCI was far less than the sizes of the subsets selected by the other methods (26 for FOCI, 45 for forward stepwise, 56 for Lasso, 51 for Dantzig selector, and 33 for SCAD). This is a recurring pattern that we saw in almost all the datasets on which we ran our tests. On rare occasions, FOCI stopped a little too soon, resulting in worse prediction errors.

Example 6.4 (Polish companies bankruptcy data). We now consider another dataset from the UCI Machine Learning Repository, known as the Polish companies bankruptcy dataset [18, 64]. The dataset consists of 19967 samples with 64 features. Each sample corresponds to a company in Poland. The response variable is binary, indicating whether or not the company was bankrupted after a period of time. We carried out the exact same comparison procedure for this data as we did for the spam data in the previous example. The results are shown Table 3. Again we see that FOCI achieved a slightly better prediction error than the other methods, but with a far fewer number of variables. FOCI selected 10 variables, whereas forward stepwise selected 24, Lasso selected 48, and the Dantzig selector selected 27. Only SCAD selected a smaller number of variables (3), but it did so at the cost of a significantly worse prediction error.

Example 6.5 (Broader comparison). In this final example, we compare the performance of FOCI with a broader set of competing methods, including methods that provide good prediction tools but are difficult or impossible to use for subset selection, such as random forests [8], mutual information [3] and SPAM [44]. We took the Polish companies bankruptcy data from Example 6.4 and divided the data randomly into training and test sets as before. For each method and each $t = 1, \ldots, 10$, we took the top $t$ variables selected by the method, fitted a predictive model using random forests, and estimated the mean squared prediction error using the test data. We took $t$ only up to 10 because we know, from Table 3, that FOCI selects the top 10
variables, and the other methods (at least four of them) do not beat that performance with a larger number of variables. The results are plotted in Figure 1. The figure shows that FOCI and random forests were by far the best methods for early detection of important variables. This is a pattern that we observed in various other examples that we analyzed while preparing this manuscript.

In our experiments, the performances of FOCI and random forests were generally similar, but FOCI has three distinct advantages over random forests: (1) FOCI selects a subset of variables, whereas random forests only give an ordering by importance and a prediction rule, (2) FOCI runs much faster than random forests in large datasets, and (3) arguably, FOCI has better theoretical support than random forests, due to the results of this paper.

7. Restatement of Theorems 2.1 and 2.2

Beginning with this section, the rest of the paper is devoted to proofs. Throughout the rest of the manuscript, whenever we say that a random variable $Y$ is a function of another variable $X$, we will mean that $Y = f(X)$ almost surely for some measurable function $f$.

First, we focus on Theorems 2.1 and 2.2. To prove these theorems, it is convenient to break up the estimators into pieces. This gives certain
‘elaborate’ versions of Theorems 2.1 and 2.2 which are interesting in their own right. First, suppose that \( p \geq 1 \). Define
\[
Q_n(Y, Z \mid X) := \frac{1}{n^2} \sum_{i=1}^{n} \left( \min\{R_i, R_{M(i)}\} - \min\{R_i, R_{N(i)}\} \right)
\]
(7.1)
and
\[
S_n(Y, X) := \frac{1}{n^2} \sum_{i=1}^{n} (R_i - \min\{R_i, R_{N(i)}\}).
\]
(7.2)
Let \( \mu \) denote the law of \( Y \). We will see later that the following theorem implies both Theorem 2.1 and Theorem 2.2 in the case \( p \geq 1 \).

**Theorem 7.1.** Suppose that \( p \geq 1 \). As \( n \to \infty \), the statistics \( Q_n(Y, Z \mid X) \) and \( S_n(Y, X) \) converge almost surely to deterministic limits. Call these limit \( a \) and \( b \), respectively. Then

(i) \( 0 \leq a \leq b \).

(ii) \( Y \) is conditionally independent of \( Z \) given \( X \) if and only if \( a = 0 \).

(iii) \( Y \) is conditionally a function of \( Z \) given \( X \) if and only if \( a = b \).

(iv) \( Y \) is not a function of \( X \) if and only if \( b > 0 \).

Explicitly, the values of \( a \) and \( b \) are given by
\[
a = \int \mathbb{E}(\text{Var}(\mathbb{P}(Y \geq t \mid Z, X) \mid X))d\mu(t)
\]
and
\[
b = \int \mathbb{E}(\text{Var}(1_{\{Y \geq t\}} \mid X))d\mu(t)
\]
\[
= \int \mathbb{E}(\mathbb{P}(Y \geq t \mid X)(1 - \mathbb{P}(Y \geq t \mid X)))d\mu(t).
\]

Next, suppose that \( p = 0 \). Define
\[
Q_n(Y, Z) := \frac{1}{n^2} \sum_{i=1}^{n} \left( \min\{R_i, R_{M(i)}\} - \frac{L_i^2}{n} \right)
\]
(7.3)
and
\[
S_n(Y) := \frac{1}{n^3} \sum_{i=1}^{n} L_i(n - L_i).
\]
(7.4)
We will prove later that the following theorem implies Theorems 2.1 and 2.2 when \( p = 0 \).

**Theorem 7.2.** As \( n \to \infty \), \( Q_n(Y, Z) \) and \( S_n(Y) \) converge almost surely to deterministic limits \( c \) and \( d \), satisfying the following properties:

(i) \( 0 \leq c \leq d \).

(ii) \( Y \) is independent of \( Z \) if and only if \( c = 0 \).

(iii) \( Y \) is a function of \( Z \) if and only if \( c = d \).

(iv) \( d > 0 \) if and only if \( Y \) not a constant.
Explicitly,
\[ c = \int \text{Var}(\mathbb{P}(Y \geq t | Z)) d\mu(t), \]
and
\[ d = \int \text{Var}(1_{\{Y \geq t\}}) d\mu(t) \]
\[ = \int \mathbb{P}(Y \geq t)(1 - \mathbb{P}(Y \geq t)) d\mu(t). \]

It is not difficult to see that when \( Y \) has a continuous distribution, \( d \) is necessarily equal to \( 1/6 \). In this case, there is no need for estimating \( d \) using \( S_n(Y, Z) \). On the other hand, the value of \( d \) may be dependent on the distribution of \( Y \) when the distribution is not continuous. In such cases, \( d \) needs to be estimated from the data using \( S_n(Y, Z) \).

8. Proofs of Theorems 2.1 and 2.2 using Theorems 7.1 and 7.2

Suppose that \( p \geq 1 \). Recall the quantities \( a \) and \( b \) from the statement of Theorem 7.1 and notice that \( T = a/b \). Suppose that \( Y \) is not a function of \( X \). Then by conclusion (iv) of Theorem 7.1 \( b > 0 \), and hence \( T \) is well-defined. Moreover, conclusion (i) implies that \( 0 \leq T \leq 1 \), conclusion (ii) implies that \( T = 0 \) if and only if \( Y \) and \( Z \) are conditionally independent given \( X \), and conclusion (iii) implies that \( Y \) is a function of \( Z \) given \( X \) if and only if \( T = 1 \). This proves Theorem 2.1 when \( p \geq 1 \). Next, note that \( T_n = Q_n/S_n \), where \( Q_n = Q_n(Y, Z|X) \) and \( S_n = S_n(Y, X) \), as defined in (7.1) and (7.2). By Theorem 7.1, \( Q_n \to a \) and \( S_n \to b \) in probability. Thus, \( T_n \to a/b = T \) in probability. This proves Theorem 2.2 when \( p \geq 1 \).

Next, suppose that \( p = 0 \). The proof proceeds exactly as before, but using Theorem 7.2. Here \( T = c/d \), where \( c \) and \( d \) are the quantities from Theorem 7.2. Suppose that \( Y \) is not a function of \( X \), which in this case just means that \( Y \) is not a constant. Then by conclusion (iv) of Theorem 7.2 \( d > 0 \), and hence \( T \) is well-defined. Moreover, conclusion (i) implies that \( 0 \leq T \leq 1 \), conclusion (ii) implies that \( T = 0 \) if and only if \( Y \) and \( Z \) are independent, and conclusion (iii) implies that \( Y \) is a function of \( Z \) if and only if \( T = 1 \). This proves Theorem 2.1 when \( p = 0 \). Next, note that \( T_n = Q_n/S_n \), where \( Q_n = Q_n(Y, Z) \) and \( S_n = S_n(Y) \), as defined in (7.3) and (7.4). By Theorem 7.2, \( Q_n \to c \) and \( S_n \to d \) in probability. Thus, \( T_n \to c/d = T \) in probability. This proves Theorem 2.2 when \( p = 0 \).

9. Preparation for the proofs of Theorems 7.1 and 7.2

In this section we prove some lemmas that are needed for the proofs of Theorems 7.1 and 7.2. Let \( Y \) be a random variable and \( X \) be an \( \mathbb{R}^p \)-valued random vector, defined on the same probability space. Define
\[ F(t) := \mathbb{P}(Y \leq t), \quad G(t) := \mathbb{P}(Y \geq t). \]
By the existence of regular conditional probabilities on regular Borel spaces (see for example [19] Theorem 2.1.15 and Exercise 5.1.16), for each Borel set $A \subseteq \mathbb{R}$ there is a measurable map $x \mapsto \mu_x(A)$ from $\mathbb{R}^p$ into $[0, 1]$, such that

(i) for any $A$, $\mu_x(A)$ is a version of $\mathbb{P}(Y \in A|X)$, and
(ii) with probability one, $\mu_x$ is a probability measure on $\mathbb{R}$.

In the above sense, $\mu_x$ is the conditional law of $Y$ given $X = x$. For each $t$, let

$$F_X(t) := \mu_x((-, t]), \quad G_X(t) := \mu_x([t, \infty)).$$

Define

$$Q(Y, X) := \int \text{Var}(G_X(t)) d\mu(t). \quad (9.1)$$

**Lemma 9.1.** Let $Q(Y, X)$ be as above. Then $Q(Y, X) = 0$ if and only if $Y$ and $X$ are independent.

*Proof.* If $Y$ and $X$ are independent, then for any $t$, $\mathbb{P}(Y \geq t|X) = \mathbb{P}(Y \geq t)$ almost surely. Thus, $G_X(t) = G(t)$ almost surely, and so $\text{Var}(G_X(t)) = 0$. Consequently, $Q(Y, X) = 0$.

Conversely, suppose that $Q(Y, X) = 0$. Then there is a set $A \subseteq \mathbb{R}$ such that $\mu(A) = 1$ and $\text{Var}(G_X(t)) = 0$ for every $t \in A$. Since $\mathbb{E}(G_X(t)) = G(t)$, $G_X(t) = G(t)$ almost surely for each $t \in A$. We claim that $A = \mathbb{R}$.

To show this, take any $t \in \mathbb{R}$. If $\mu(\{t\}) > 0$, then clearly $t$ must be a member of $A$ and there is nothing more to prove. So assume that $\mu(\{t\}) = 0$.

This implies that $G$ is right-continuous at $t$.

There are two possibilities. First, suppose that $G(s) < G(t)$ for all $s > t$. Then for each $s > t$, $\mu([t, s)) > 0$, and hence $A$ must intersect $[t, s)$. This shows that there is a sequence $r_n$ in $A$ such that $r_n$ decreases to $t$. Since $G_X(r_n) = G(r_n)$ almost surely for each $n$, this implies that with probability one,

$$G_X(t) \geq \lim_{n \to \infty} G_X(r_n) = \lim_{n \to \infty} G(r_n) = G(t).$$

But $\mathbb{E}(G_X(t)) = G(t)$. Thus, $G_X(t) = G(t)$ almost surely.

The second possibility is that there is some $s > t$ such that $G(s) = G(t)$. Take the largest such $s$, which exists because $G$ is left-continuous. If $s = \infty$, then $G(t) = G(s) = 0$, and hence $G_X(t) = 0$ almost surely because $\mathbb{E}(G_X(t)) = G(t)$. Suppose that $s < \infty$. Then either $\mu(\{s\}) > 0$, which implies that $G_X(s) = G(s)$ almost surely, or $\mu(\{s\}) = 0$ and $G(r) < G(s)$ for all $r > s$, which again implies that $G_X(s) = G(s)$ almost surely, by the previous paragraph. Therefore in either case, with probability one,

$$G_X(t) \geq G_X(s) = G(s) = G(t).$$

Since $\mathbb{E}(G_X(t)) = G(t)$, this implies that $G_X(t) = G(t)$ almost surely.

This completes the proof of our claim that $\text{Var}(G_X(t)) = 0$ for every $t \in \mathbb{R}$. In particular, for each $t \in \mathbb{R}$, $G_X(t) = G(t)$ almost surely. Therefore,
for any $t \in \mathbb{R}$ and any Borel set $B \subseteq \mathbb{R}^q$,

$$\mathbb{P}(\{Y \geq t\} \cap \{X \in B\}) = \mathbb{E}(\mathbb{P}(Y \geq t|X) 1_{X \in B})$$

$$= G(t)\mathbb{P}(X \in B) = \mathbb{P}(Y \geq t)\mathbb{P}(X \in B).$$

This proves that $Y$ and $X$ are independent. \qed

Let $Z$ be an $\mathbb{R}^q$-valued random vector defined on the same probability space as $Y$ and $X$, and let $W = (X, Z)$ be the concatenation of $X$ and $Z$.

**Lemma 9.2.** Let $W$ be as above. Then $Q(Y, W) \geq Q(Y, X)$, and equality holds if and only if $Y$ and $Z$ are conditionally independent given $X$.

**Proof.** Since $G_X(t) = \mathbb{E}(G_W(t)|X)$, it follows that for each $t$,

$$\text{Var}(G_X(t)) \leq \text{Var}(G_W(t)).$$

Consequently, $Q(Y, W) \geq Q(Y, X)$. If $Y$ and $Z$ are conditionally independent given $X$, then for any $t$,

$$G_W(t) = \mathbb{P}(Y \geq t|X, Z) = \mathbb{P}(Y \geq t|X) = G_X(t).$$

Therefore, $Q(Y, W) = Q(Y, X)$. Conversely, suppose that $Q(Y, W) = Q(Y, X)$. Notice that

$$\text{Var}(G_W(t)) - \text{Var}(G_X(t)) = \text{Var}(G_W(t)) - \mathbb{E}(\mathbb{E}(G_W(t)|X))$$

$$= \mathbb{E}(\text{Var}(G_W(t)|X))$$

$$= \mathbb{E}(G_W(t) - G_X(t))^2.$$

Thus,

$$Q(Y, W) - Q(Y, X) = \int \mathbb{E}(G_W(t) - G_X(t))^2 d\mu(t).$$

So, if $Q(Y, W) = Q(Y, X)$, then there is a Borel set $A \subseteq \mathbb{R}$ such that $\mu(A) = 1$ and $G_W(t) = G_X(t)$ almost surely for every $t \in A$. We claim that $A = \mathbb{R}$. Let us now prove this claim. The proof is similar to the proof of the analogous claim in Lemma 9.1 with a few additional complications.

Take any $t \in \mathbb{R}$. If $\mu(\{t\}) > 0$, then clearly $t$ must be a member of $A$. So assume that $\mu(\{t\}) = 0$. As before, this implies that $G$ is right-continuous at $t$. Take any sequence $t_n$ decreasing to $t$. Then $G(t) - G(t_n) \to 0$. But

$$G(t) - G(t_n) = \mathbb{E}(G_X(t) - G_X(t_n)),$$

and $G_X(t) - G_X(t_n)$ is a nonnegative random variable. Thus, $G_X(t) - G_X(t_n) \to 0$ in probability, and therefore there is a subsequence $n_k$ such that $G_X(t_{n_k})$ converges to $G_X(t)$ almost surely. But from the properties of the regular conditional probability $\mu_X$ we know that $G_X$ is a non-increasing function almost surely. Thus, it follows that $G_X$ is right-continuous at $t$ almost surely.

Now, as before, there are two possibilities. First, suppose that $G(s) < G(t)$ for all $s > t$. Then for each $s > t$, $\mu([t, s)) > 0$, and hence $A$ must intersect $[t, s)$. This shows that there is a sequence $r_n$ in $A$ such that $r_n$ decreases to $t$. Since $G_W(r_n) = G_X(r_n)$ almost surely for each $n$ and $G_X$ is
right-continuous at $t$ with probability one, this implies that with probability one,
\[ G_W(t) \geq \lim_{n \to \infty} G_W(r_n) = \lim_{n \to \infty} G_X(r_n) = G_X(t). \]

But $\mathbb{E}(G_W(t) | X) = G_X(t)$. Thus, $G_W(t) = G_X(t)$ almost surely.

The second possibility is that there is some $s > t$ such that $G(s) = G(t)$. Take the largest such $s$, which exists because $G$ is left-continuous. If $s = \infty$, then $G(t) = G(s) = 0$, and hence $G_W(t) = G_X(t) = 0$ almost surely because $\mathbb{E}(G_W(t)) = \mathbb{E}(G_X(t)) = G(t)$. Suppose that $s < \infty$. Then either $\mu(\{s\}) > 0$, which implies that $G_W(s) = G_X(s)$ almost surely (by the previous step), or $\mu(\{s\}) = 0$ and $G(r) < G(s)$ for all $r > s$, which again implies that $G_W(s) = G_X(s)$ almost surely (also by the previous step). Therefore in either case, with probability one,
\[ G_W(t) \geq G_W(s) = G_X(s). \]

Now, $\mathbb{P}(Y \in [t, s]) = 0$, and hence $\mathbb{P}(Y \in [t, s] | X) = 0$ almost surely. In other words, $G_X(t) = G_X(s)$ almost surely. Thus, $G_W(t) \geq G_X(s)$ almost surely. Since $\mathbb{E}(G_W(t) | X) = G_X(t)$, this implies that $G_W(t) = G_X(t)$ almost surely. This completes the proof of our claim that $A = \mathbb{R}$.

Therefore, for any $t \in \mathbb{R}$ and any Borel set $B \subseteq \mathbb{R}^d$,
\[
\mathbb{P}(\{Y \geq t\} \cap \{Z \in B\} | X) = \mathbb{E}(\mathbb{P}(\{Y \geq t\} \cap \{Z \in B\} | Z) | X)
= \mathbb{E}(\mathbb{P}(Y \geq t | W) 1_{\{Z \in B\}} | X)
= \mathbb{E}(G_X(t) 1_{\{Z \in B\}} | X)
= \mathbb{P}(Y \geq t | X) \mathbb{P}(Z \in B | X).
\]

This proves that $Y$ and $Z$ are conditionally independent given $X$. \hfill \Box

Let $X_1, X_2, \ldots$ be an infinite sequence of i.i.d. copies of $X$. For each $n \geq 2$ and each $1 \leq i \leq n$, let $X_{n,i}$ be the Euclidean nearest-neighbor of $X_i$ among $\{X_j : 1 \leq j \leq n, j \neq i\}$. Ties are broken at random.

**Lemma 9.3.** With probability one, $X_{n,1} \to X_1$ as $n \to \infty$.

**Proof.** Let $\nu$ be the law of $X$. Let $A$ be the support of $\nu$. Recall that $A$ is the set of all $x \in \mathbb{R}^p$ such that any open ball containing $x$ has strictly positive $\nu$-measure. From this definition it follows easily that the complement of $A$ is a countable union of open balls of $\nu$-measure zero. Consequently, $X \in A$ with probability one.

Take any $\varepsilon > 0$. Let $B$ be the ball of radius $\varepsilon$ centered at $X_1$. Then
\[
\mathbb{P}(\|X_1 - X_{n,1}\| \geq \varepsilon | X_1) \leq (1 - \nu(B))^{n-1}
\]
Since $X_1 \in A$ almost surely, it follows that $\nu(B) > 0$ almost surely. Thus,
\[
\lim_{n \to \infty} \mathbb{P}(\|X_1 - X_{n,1}\| \geq \varepsilon | X_1) = 0
\]
amt surely, and hence
\[
\lim_{n \to \infty} \mathbb{P}(\|X_1 - X_{n,1}\| \geq \varepsilon) = 0.
\]
This proves that \( \|X_1 - X_n,1\| \to 0 \) in probability. But \( \|X_1 - X_n,1\| \) is decreasing in \( n \). Therefore \( \|X_1 - X_n,1\| \to 0 \) almost surely. \( \square \)

Take any particular realization of \( X_1, \ldots, X_n \). In this realization, for each \( 1 \leq i \leq n \), let \( K_{n,i} \) be the number of \( j \) such that \( X_i \) is a nearest neighbor of \( X_j \) (not necessarily the randomly chosen one) and \( X_j \neq X_i \). The following is a well-known geometric fact (see for example [62, page 102]).

**Lemma 9.4.** There is a deterministic constant \( C(p) \), depending only on the dimension \( p \), such that \( K_{n,1} \leq C(p) \) always.

**Proof.** Consider a triangle with vertices \( x, y, \) and \( z \) in \( \mathbb{R}^p \), where \( y \neq x \) and \( z \neq x \). Suppose that the angle at \( x \) is strictly less than 60° and \( \|y - x\| \leq \|x - z\| \). Then

\[
\frac{(y - x) \cdot (z - x)}{\|y - x\| \|z - x\|} > \cos 60° = \frac{1}{2}.
\]

Consequently,

\[
\|z - y\|^2 = \|z - x\|^2 + \|x - y\|^2 + 2(z - x) \cdot (x - y) < \|z - x\|^2 + \|x - y\|^2 - \|y - x\| \|z - x\| \leq \|z - x\|^2,
\]

where the last inequality holds because \( \|x - y\| \leq \|x - z\| \). Thus, if \( K \) is a cone at \( x \) of aperture less than 60°, and \( x_1, \ldots, x_m \) is a finite list of points in \( K \setminus \{x\} \) (not necessarily distinct), then there can be at most one \( i \) such that the nearest neighbor of \( x_i \) in \( \{x, x_1, \ldots, x_m\} \) is \( x \).

Now, it is not difficult to see that there is a deterministic constant \( C(p) \) depending only on \( p \) such that the whole of \( \mathbb{R}^p \) can be covered by at most \( C(p) \) cones of apertures less than 60° based at any given point. Take this point to be \( X_1 \). Then within each cone, there can be at most one \( X_j \), which is not equal to \( X_1 \), and whose nearest neighbor is \( X_1 \). This shows that there can be at most \( C(p) \) points distinct from \( X_1 \) whose nearest neighbor is \( X_1 \), completing the proof of the lemma. \( \square \)

**Lemma 9.5.** There is a constant \( C(p) \) depending only on \( p \), such that for any measurable \( f : \mathbb{R}^p \to [0, \infty) \) and any \( n \), \( \mathbb{E}(f(X_{n,1})) \leq C(p)\mathbb{E}(f(X_1)) \).

**Proof.** Since \( f \) is nonnegative,

\[
\mathbb{E}(f(X_{n,i})) \leq \mathbb{E}(f(X_i)) + \mathbb{E}(f(X_{n,i})1_{\{X_{n,i} \neq X_i\}}) \\
\leq \mathbb{E}(f(X_i)) + \sum_{j=1}^{n} \mathbb{E}(f(X_j)1_{\{X_j = X_{n,i}, X_j \neq X_i\}}).
\]
Therefore by symmetry,
\[
\mathbb{E}(f(\mathbf{X}_{n,1})) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}(f(\mathbf{X}_{n,i}))
\]
\[
\leq \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}(f(\mathbf{X}_i)) + \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbb{E}(f(\mathbf{X}_j)\mathbb{1}_{\mathbf{X}_j = \mathbf{X}_{n,i} \land \mathbf{X}_j \neq \mathbf{X}_i})
\]
\[
= \mathbb{E}(f(\mathbf{X}_1)) + \frac{1}{n} \sum_{j=1}^{n} \mathbb{E}\left(f(\mathbf{X}_j) \sum_{i=1}^{n} \mathbb{1}_{\mathbf{X}_j = \mathbf{X}_{n,i} \land \mathbf{X}_j \neq \mathbf{X}_i}\right)
\]
\[
\leq \mathbb{E}(f(\mathbf{X}_1)) + \frac{1}{n} \sum_{j=1}^{n} \mathbb{E}(f(\mathbf{X}_j)K_{n,j}) = \mathbb{E}(f(\mathbf{X}_1)(1 + K_{n,1})).
\]

By Lemma 9.4, this completes the proof. □

For the next result, we will need the following version of Lusin’s theorem (proved, for example, by combining [45, Theorem 2.18 and Theorem 2.24]).

**Lemma 9.6** (Special case of Lusin’s theorem). Let \( f : \mathbb{R}^p \to \mathbb{R} \) be a measurable function and \( \gamma \) be a probability measure on \( \mathbb{R}^p \). Then, given any \( \varepsilon > 0 \), there is a compactly supported continuous function \( g : \mathbb{R}^p \to \mathbb{R} \) such that
\[
\gamma(\{ \mathbf{x} : f(\mathbf{x}) \neq g(\mathbf{x}) \}) < \varepsilon.
\]

**Lemma 9.7.** For any measurable \( f : \mathbb{R}^p \to \mathbb{R} \), \( f(\mathbf{X}_1) - f(\mathbf{X}_{n,1}) \) tends to 0 in probability as \( n \to \infty \).

**Proof.** Fix some \( \varepsilon > 0 \). Let \( g \) be a function as in Lemma 9.6, for the given \( f \) and \( \varepsilon \), and \( \gamma = \text{the law of } \mathbf{X}_1 \). Then note that for any \( \delta > 0 \),
\[
\mathbb{P}(|f(\mathbf{X}_1) - f(\mathbf{X}_{n,1})| > \delta)
\]
\[
\leq \mathbb{P}(|g(\mathbf{X}_1) - g(\mathbf{X}_{n,1})| > \delta) + \mathbb{P}(f(\mathbf{X}_1) \neq g(\mathbf{X}_1))
\]
\[
+ \mathbb{P}(f(\mathbf{X}_{n,1}) \neq g(\mathbf{X}_{n,1})).
\]

By Lemma 9.3 and the continuity of \( g \),
\[
\lim_{n \to \infty} \mathbb{P}(|g(\mathbf{X}_1) - g(\mathbf{X}_{n,1})| > \delta) = 0.
\]

By the construction of \( g \),
\[
\mathbb{P}(f(\mathbf{X}_1) \neq g(\mathbf{X}_1)) < \varepsilon.
\]

Finally, by Lemma 9.5,
\[
\mathbb{P}(f(\mathbf{X}_{n,1}) \neq g(\mathbf{X}_{n,1})) \leq C(p)\mathbb{P}(f(\mathbf{X}_1) \neq g(\mathbf{X}_1)) \leq C(p)\varepsilon.
\]

Putting it all together, we get
\[
\limsup_{n \to \infty} \mathbb{P}(|f(\mathbf{X}_1) - f(\mathbf{X}_{n,1})| > \delta) \leq \varepsilon + C(p)\varepsilon.
\]

Since \( \varepsilon \) and \( \delta \) are arbitrary, this completes the proof of the lemma. □
Let \((Y_1, X_1), \ldots, (Y_n, X_n)\) be i.i.d. copies of \((Y, X)\). Let \(F_n\) be the empirical distribution function of \(Y_1, \ldots, Y_n\), that is, 
\[
F_n(t) = \frac{1}{n} \sum_{i=1}^{n} 1\{Y_i \leq t\}.
\]
Also let 
\[
G_n(t) = \frac{1}{n} \sum_{i=1}^{n} 1\{Y_i \geq t\}.
\]
For each \(i\), let \(N(i)\) be the index \(j\) such that \(X_j = X_{n,i}\) (ties broken at random). Define 
\[
Q_n = Q_n(Y, X) := \frac{1}{n} \sum_{i=1}^{n} \left( \min\{F_n(Y_i), F_n(Y_{N(i)})\} - G_n(Y_i)^2 \right).
\]
Note that this is exactly the statistic \(Q_n(Y, X)\) defined in equation (7.3) of Section 7.

**Lemma 9.8.** Let \(Q_n\) be defined as above. Then 
\[
\lim_{n \to \infty} \mathbb{E}(Q_n(Y, X)) = Q(Y, X).
\]

**Proof.** Let 
\[
Q'_n := \frac{1}{n} \sum_{i=1}^{n} \left( \min\{F(Y_i), F(Y_{N(i)})\} - G(Y_i)^2 \right).
\]
and let 
\[
\Delta_n := \sup_{t \in \mathbb{R}} |F_n(t) - F(t)| + \sup_{t \in \mathbb{R}} |G_n(t) - G(t)|.
\]
Then by the triangle inequality, 
\[
|Q'_n - Q_n| \leq 3\Delta_n. \tag{9.2}
\]
On the other hand, by the Glivenko–Cantelli theorem, \(\Delta_n \to 0\) almost surely as \(n \to \infty\). Since \(\Delta_n\) is bounded by 2, this implies that 
\[
\lim_{n \to \infty} \mathbb{E}|Q'_n - Q_n| = 0.
\]
Thus, it suffices to show that \(\mathbb{E}(Q'_n)\) converges to \(Q(Y, X)\). First, notice that 
\[
\min\{F(Y_1), F(Y_{N(1)})\} = \int 1_{\{Y_1 \geq t\}} 1_{\{Y_{N(1)} \geq t\}} d\mu(t).
\]
Let \(\mathcal{F}\) be the \(\sigma\)-algebra generated by \(X_1, \ldots, X_n\) and the random variables used for breaking ties in the selection of nearest neighbors. Then for any \(t\), 
\[
\mathbb{E}(1_{\{Y_1 \geq t\}} 1_{\{Y_{N(1)} \geq t\}} | \mathcal{F}) = G_{X_1}(t) G_{X_{N(1)}}(t).
\]
Note that \(X_{N(1)} = X_{n,1}\). Also, recall that by the properties of the regular conditional probability \(\mu_x\), the map \(x \mapsto G_x(t)\) is measurable. Therefore by the above identity and Lemma 9.7, we have 
\[
\lim_{n \to \infty} \mathbb{E}(1_{\{Y_1 \geq t\}} 1_{\{Y_{N(1)} \geq t\}}) = \mathbb{E}(G_X(t)^2).
\]
Thus, 
\[ \lim_{n \to \infty} \mathbb{E}(Q'_n) = \int (\mathbb{E}(G_X(t)^2) - G(t)^2) d\mu(t). \]
Since \( \mathbb{E}(G_X(t)) = G(t) \), this completes the proof of the lemma. \( \square \)

**Lemma 9.9.** There are positive constants \( C_1 \) and \( C_2 \) depending only on the dimension \( p \) such that for any \( n \) and any \( t \geq 0 \),
\[ \mathbb{P}(|Q_n - \mathbb{E}(Q_n)| \geq t) \leq C_1 e^{-C_2 n t^2}. \]

**Proof.** Throughout this proof, \( C(p) \) will denote any constant that depends only on \( p \). The value of \( C(p) \) may change from line to line.

In addition to the variables \( X_i \) and \( Y_i \), in this proof we will make use of i.i.d. Uniform\([0,1]\) random variables \( U_1, \ldots, U_n \), where \( U_i \) is used for breaking ties if \( X_i \) has multiple nearest neighbors.

Our plan is to use the bounded difference concentration inequality \[39\]. For that, we have to get a bound on the maximum possible change in \( Q_n \) if one \((Y_i, X_i, U_i)\) is replaced by some alternative value \((Y'_i, X'_i, U'_i)\). We first write \( Q_n = A_n + B_n \), where
\[ A_n := \frac{1}{n} \sum_{i=1}^{n} \min\{F_n(Y_i), F_n(Y_{N(i)})\}, \quad B_n := \frac{1}{n} \sum_{i=1}^{n} G_n(Y_i)^2. \]

It is not hard to see that after the above replacement, each \( G_n(Y_j) \) can change by at most \( 1/n \), and since these quantities are in \([0,1]\), \( B_n \) can change by at most \( 2/n \). Therefore the bounded difference inequality gives
\[ \mathbb{P}(|B_n - \mathbb{E}(B_n)| \geq t) \leq 2e^{-nt^2/8}. \quad (9.3) \]

Unfortunately, \( A_n \) is not well-behaved with respect to this kind of perturbation, so we have to first replace \( A_n \) by some more manageable quantity. Take a realization of \((Y_1, X_1, U_1), \ldots, (Y_n, X_n, U_n)\). Define an equivalence relation on \( \{1, \ldots, n\} \) by declaring that \( i \) and \( j \) are equivalent if \( X_i = X_j \). Call an equivalence class a ‘cluster’ if its size is greater than one, and a ‘singleton’ otherwise. Note that if \( i \) belongs to a cluster \( \mathcal{C} \), then \( N(i) \) must necessarily be also a member of the same cluster. In fact, \( N(i) \) would be chosen uniformly at random (using \( U_i \)) from \( \mathcal{C} \setminus \{i\} \).

Let \( \mathcal{C} \) denote the set of all clusters and \( \mathcal{S} \) denote the set of all singletons. For convenience, let us define
\[ a_{i,j} := \min\{F_n(Y_i), F_n(Y_j)\}, \]
so that
\[ A_n = \frac{1}{n} \sum_{\mathcal{C} \in \mathcal{C}} \sum_{i \in \mathcal{C}} a_{i,N(i)} + \frac{1}{n} \sum_{i \in \mathcal{S}} a_{i,N(i)}. \]
Let $G$ denote the $\sigma$-algebra generated by $(Y_1, X_1), \ldots, (Y_n, X_n)$ and $(U_i)_{i \in S}$. Define $A'_n := \mathbb{E}(A_n | G)$. Then it is clear that

$$A'_n = \frac{1}{n} \sum_{C \in \mathcal{C}} b(C) + \frac{1}{n} \sum_{i \in S} a_{i, N(i)}, \quad (9.4)$$

where

$$b(C) := \frac{1}{|C|-1} \sum_{i \in C} \sum_{j \in C \setminus \{i\}} a_{i,j}.$$  

We will now use the bounded difference inequality to get a tail bound for the difference $A_n - A'_n$. Conditional on $G$, $A_n$ is a function of $(U_i)_{i \in S}$. If one such $U_i$ is replaced by some other value $U'_i$, then only $N(i)$ may be affected. Thus, $A_n$ changes by at most $1/n$. Therefore, the bounded difference inequality gives

$$\mathbb{P}(|A_n - A'_n| \geq t | G) \leq 2e^{-nt^2/2}.$$  

Since the right side is deterministic, we can remove the conditioning on the left. But then the tail bound gives $\mathbb{E}|A_n - A'_n| < 3n^{-1/2}$. Therefore,

$$\mathbb{P}(|A_n - \mathbb{E}(A_n)| \geq 3n^{-1/2} + t)$$

$$\leq \mathbb{P}(|A_n - A'_n| \geq t/2) + \mathbb{P}(|A'_n - \mathbb{E}(A'_n)| \geq t/2)$$

$$\leq 2e^{-nt^2/8} + \mathbb{P}(|A'_n - \mathbb{E}(A'_n)| \geq t/2). \quad (9.5)$$

So we now need to get a tail bound for $A'_n - \mathbb{E}(A'_n)$. Fortunately, $A'_n$ is well-behaved with respect to perturbing one coordinate. Let us now try to figure out the maximum possible change in $A'_n$ if some $(Y_i, X_i, U_i)$ is replaced by an alternative value $(Y'_i, X'_i, U'_i)$. We will do this in stages. First, let us replace $X_i$ by $X'_i$, keeping $Y_i$ and $U_i$ fixed. We know by Lemma 9.4 that in any configuration, for any $i$ there can be at most $C(p)$ singletons $j$ such that $i$ is a nearest neighbor of $j$ (not necessarily the chosen one). This fact will be used many times in the following argument. There are several cases to consider:

1. Suppose that $i$ is in some cluster $C$ of size $\geq 3$ in the original configuration, and lands up in some other cluster $C'$ in the new configuration. Then the set of singletons is the same in the two configurations. If $j$ is a singleton, then $N(j)$ can change only if $i$ is a nearest neighbor of $j$ in either the original configuration or the final configuration. As noted above, there can be at most $C(p)$ such $j$. Therefore, due to these changes, $A'_n$ can change by at most $C(p)/n$. On the other
hand, $b(C)$ changes by at most 1, as seen from the following computation:

$$|b(C) - b(C \setminus \{i\})| = \left| \frac{1}{|C| - 1} \sum_{j \in C} \sum_{k \in C \setminus \{j\}} a_{j,k} - \frac{1}{|C| - 2} \sum_{j \in C \setminus \{i\}} \sum_{k \in C \setminus \{i,j\}} a_{j,k} \right|
$$

$$= \left| \frac{1}{|C| - 1} \sum_{k \in C \setminus \{i\}} a_{i,k} - \frac{1}{(|C| - 1)(|C| - 2)} \sum_{j \in C \setminus \{i\}} \sum_{k \in C \setminus \{i,j\}} a_{j,k} \right| \leq 1,$$

where the last inequality holds because the $a_{i,j}$'s are in $[0, 1]$. A similar calculation shows that $b(C')$ also changes by at most 1. Thus, overall, $A'_n$ changes by at most $C(p)/n$.

(2) Suppose that $i$ is in some cluster $C$ of size $\geq 3$ in the original configuration, and pairs up with a singleton to form a new cluster in the new configuration. Again, $b(C)$ changes by at most 1, and the contributions from the singletons in (9.4) changes by at most $C(p)/n$, by the same logic as in case (1). The formation of the new cluster causes a change of at most $2/n$. Therefore, again, the change in $A'_n$ is at most $C(p)/n$.

(3) Suppose that $i$ is in some cluster $C$ of size $\geq 3$ in the original configuration, and becomes a singleton in the new configuration. Then just as before, $b(C)$ changes by at most 1, and the contributions from singletons changes by at most $C(p)/n$.

(4) Suppose that $i$ is in some cluster $C$ of size 2 in the original configuration, and pairs up with a singleton to form a new cluster in the new configuration. Again, the number of singletons $j$ for which $N(j)$ changes due to this operation is bounded by $C(p)$, and the contributions from the clusters terms in (9.4) also changes by at most a bounded amount. Thus, the change in $A'_n$ is at most $C(p)/n$.

(5) Suppose that $i$ is in some cluster $C$ of size 2 in the original configuration, and becomes a singleton in the new configuration. Proceeding as before, we see that $A'_n$ changes by at most $C(p)/n$.

(6) Suppose that $i$ is a singleton in the original configuration and remains so in the new configuration. Again, it is clear that the change in $A'_n$ is at most $C(p)/n$.

(7) All other cases are just reverses of the situations considered above. For example, if $i$ is a singleton in the original configuration and becomes part of a cluster of size $\geq 3$ in the new configuration, that’s just the reverse of case (3).

Thus, we conclude that changing $X_i$ to $X'_i$ changes $A'_n$ by at most $C(p)/n$. Next, let us change $Y_i$ to $Y'_i$. Then $F_n(Y'_j)$ changes by at most $1/n$ for each $j \neq i$, and $F_n(Y'_i)$ changes by at most 1. Therefore each $a_{j,k}$ changes by at most $1/n$ if $j \neq i$ and $k \neq i$, and by at most 1 if either index equals $i$. From this it is easy to see that $A'_n$ can change by at most $1/n$. Finally, let us
replace $U_i$ by $U'_i$. Then only $N(i)$ can change, and hence $A'_n$ can change by at most $1/n$. Combing all three steps, we get

$$\mathbb{P}(|A'_n - \mathbb{E}(A'_n)| \geq t) \leq 2e^{-C(p)n^{t^2}}.$$  

Therefore by (9.3) and (9.5), we get

$$\mathbb{P}(|A_n - \mathbb{E}(A_n)| \geq 3n^{-1/2} + t) \leq 6e^{-C(p)n^{t^2}}.$$  

If $t \geq 3n^{-1/2}$, this bound holds for $\mathbb{P}(|A_n - \mathbb{E}(A_n)| \geq 2t)$. If $t < 3n^{-1/2}$, we can choose $C_1 \geq 6$ so that $C_1e^{-C(p)n^{t^2}} \geq 1$, so that it is trivially a bound for $\mathbb{P}(|A_n - \mathbb{E}(A_n)| \geq 2t)$. This completes the proof.

Combining Lemmas 9.8 and 9.9, we get the following corollary.

**Corollary 9.10.** As $n \to \infty$, $Q_n(Y, X) \to Q(Y, X)$ almost surely.

10. **Proof of Theorem 7.2**

Note that convergence of $Q_n(Y, Z)$ to the deterministic limit $c$ is the result of Corollary 9.10 (applied to the pair $(Y, Z)$ instead of $(Y, X)$). Showing that $S_n(Y)$ converges to $d$ is easier. Let

$$S'_n(Y) = \frac{1}{n} \sum_{i=1}^{n} G(Y_i)(1 - G(Y_i)),$$

and

$$\Delta_n := \sup_{t \in \mathbb{R}} |G_n(t) - G(t)|.$$  

Then by triangle inequality $|S_n(Y) - S'_n(Y)| \leq 4\Delta_n$, and by the Glivenko–Cantelli theorem $\Delta_n \to 0$ almost surely. So it is enough to show that $S'_n(Y)$ converges almost surely to $d$. But that is a consequence of the strong law of large numbers, since the $Y_i$'s are i.i.d and

$$\mathbb{E}(G(Y_i)(1 - G(Y_i))) = \int G(t)(1 - G(t))d\mu(t) = d.$$  

This completes the proof of the convergence claims in the theorem. Next, by combining Corollary 9.10 and Lemma 9.1, we see that if $Y$ and $X$ are independent, then $c = 0$. This proves claim (i) in the theorem. On the other hand, if $Y$ is a function of $Z$, say $Y = f(Z)$ almost surely, then

$$c = \int \text{Var}(\mathbb{P}(Y \geq t|Z))d\mu(t)$$

$$= \int \text{Var}(\mathbb{E}(1_{\{Y \geq t\}}|Z))d\mu(t)$$

$$= \int \text{Var}(1_{\{f(Z) \geq t\}})d\mu(t)$$

$$= \int \mathbb{E}(1_{\{f(Z) \geq t\}})(1 - \mathbb{E}(1_{\{f(Z) \geq t\}}))d\mu(t) = d.$$
which proves claim (ii) in the theorem. Finally, by the law of total variance we have

\[ \text{Var}(1_{\{Y \geq t\}}) = \mathbb{E}(\text{Var}(1_{\{Y \geq t\}} | Z)) + \text{Var}(\mathbb{P}(Y \geq t | Z)), \]

therefore \(0 \leq c \leq d\). Note that by Lemma 9.1, \(c = 0\) if and only if \(Y\) is independent of \(Z\). To complete the proof of claim (iii), we have to show that if \(c = d\) then \(Y\) is almost surely a function of \(Z\). If \(c = d\), then

\[ \int \mathbb{E}(G_Z(t) - G_Z(t)^2) d\mu(t) = 0, \]

which implies that \(\mathbb{P}(E) = 1\), where \(E\) is the event

\[ \int G_Z(t)(1 - G_Z(t)) d\mu(t) = 0. \tag{10.1} \]

Let \(A\) be the support of \(\mu\). Define

\[ a_Z := \sup\{t : G_Z(t) = 1\}, \quad b_Z := \inf\{t : G_Z(t) = 0\}, \]

so that \(a_Z \leq b_Z\). Now suppose that the event \(\{a_Z < b_Z\} \cap E\) takes place. Since \(G_Z(t) \in (0, 1)\) for all \(t \in (a_Z, b_Z)\), the condition \(\text{Var}(G_Z(t)) = 0\). Since \((a_Z, b_Z)\) is an open interval, this implies that \((a_Z, b_Z) \subseteq A^c\). On the other hand, under the given circumstance, we also have \(\mathbb{P}(Y \in (a_Z, b_Z) | Z) > 0\). Thus \(\mathbb{P}(Y \in A^c | Z) = 1\). Therefore \(a_Z = b_Z = 1\). This implies that \(Y\) is almost surely a function of \(Z\).

11. Proof of Theorem 7.1

For the proof of Theorem 7.1, we need some additional lemmas.

**Lemma 11.1.** Let \(Q_n(Y, Z | X)\) be defined as in (7.1). Then \(Q_n(Y, Z | X)\) converges to \(Q(Y, Z | X)\) almost surely as \(n \to \infty\), where

\[ Q(Y, Z | X) := \int \mathbb{E}(\text{Var}(G_W(t) | X)) d\mu(t), \]

where, as before, \(W = (X, Z)\).

**Proof.** Note that \(Q_n(Y, Z | X) = Q_n(Y, W) - Q_n(Y, X)\). Also,

\[ \mathbb{E}(G_W(t) | X) = G_X(t), \]

which, by the law of total variance, gives

\[ \text{Var}(G_W(t)) - \text{Var}(G_X(t)) = \mathbb{E}(\text{Var}(G_W(t) | X)). \]

Thus,

\[ Q(Y, Z | X) = Q(Y, W) - Q(Y, X). \]

The result now follows by Corollary 9.10.
Lemma 11.2. For $S_n(Y, X)$ defined in (7.2),

$$\lim_{n \to \infty} \mathbb{E}(S_n(Y, X)) = S(Y, X)$$

where $S(Y, X) := \int \mathbb{E}(\text{Var}(1_{Y \geq t}|X))d\mu(t)$.

Proof. The proof uses techniques developed for the proof of Lemma 9.8. Let

$$S'_n(Y, X) = \frac{1}{n} \sum_{i=1}^{n} (F(Y_i) - \min\{F(Y_i), F(Y_{N(i)})\}),$$

and

$$\Delta_n := \sup_{t \in \mathbb{R}} |F_n(t) - F(t)|.$$

By the triangle inequality,

$$|S'_n(Y, X) - S_n(Y, X)| \leq 4\Delta_n.$$

By the Glivenko–Cantelli theorem, $\Delta_n \to 0$ almost surely and since $\Delta_n$ is bounded by 1, we can conclude that,

$$\lim_{n \to \infty} \mathbb{E}|S'_n(Y, X) - S_n(Y, X)| = 0.$$

Then it is enough to show that $\mathbb{E}(S'_n(Y, X))$ converges to $S(Y, X)$. Proceeding as in the proof of Lemma 9.8 we get

$$\lim_{n \to \infty} \mathbb{E}(S'_n(Y, X)) = \int (G(t) - \mathbb{E}(G(t)^2))d\mu(t)$$

$$= \int \mathbb{E}(G_X(t) - G_X(t)^2)d\mu(t) = S(Y, X),$$

which completes the proof. \[\square\]

Lemma 11.3. There are positive constants $C_1$ and $C_2$ depending only on $p$ such that for any $n$ and any $t \geq 0$,

$$\mathbb{P}(|S_n(Y, X) - \mathbb{E}(S_n(Y, X))| \geq t) \leq C_1 e^{-C_2nt^2}.$$

Proof. The concentration for the second term in the definition (7.2) was already argued in the proof of Lemma 9.9. For the first term, a simple application of the bounded difference inequality suffices. \[\square\]

Finally, we are ready to prove Theorem 7.1

Proof of Theorem 7.1. Convergence of $Q_n(Y, Z|X)$ almost surely to $a = Q(Y, Z|X)$ is the content of Lemma 11.1 and convergence of $S_n(Y, X)$ to $b = S(Y, X)$ follows by Lemmas 11.2 and 11.3.

Let us now prove the claims (i), (ii) and (iii) of the theorem. First, let us prove (i). It is not hard to see that $a = Q(Y, W) - Q(Y, X)$. Thus if $Y$ and
\( Z \) are conditionally independent given \( X \), then by Lemma 9.2, \( a = 0 \). This proves (i). Next, note that
\[
b - a = \int \mathbb{E}(\text{Var}(1_{\{Y \geq t\}}|X) - \text{Var}(\mathbb{E}(1_{\{Y \geq t\}}|Z, X)|X)) d\mu(t)
\]
\[
= \int \mathbb{E}(\text{Var}(1_{\{Y \geq t\}}|Z, X)) d\mu(t)
\]
\[
= \int \mathbb{E}(\text{Var}(1_{\{Y \geq t\}}|Z)) d\mu(t).
\]

Now, if with probability one \( Y \) is a function of \( Z \) conditional on \( X \), then \( \text{Var}(1_{\{Y \geq t\}}|Z, X) = 0 \) almost surely. Thus, the above expression shows that \( a = b \) in this situation.

Finally, let us prove claim (iii). Note that the above expression for \( b - a \) also shows that \( 0 \leq a \leq b \), since \( \text{Var}(1_{\{Y \geq t\}}|Z, X) \geq 0 \). Thus, it suffices to prove the opposite implications for (i) and (ii).

If \( a = 0 \), then again by Lemma 9.2 we get that \( Y \) and \( Z \) are conditionally independent given \( X \). If \( a = b \), then there exists a set \( A \subseteq \mathbb{R} \) such that \( \mu(A) = 1 \) and for any \( t \in A \) we have
\[
\text{Var}(1_{\{Y \geq t\}}|Z, X) = 0
\]
almost surely. Proceeding as the last part of the proof of Theorem 7.2, we can now conclude that \( Y \) is almost surely equal to a function of \( W \). This implies that \( Y \) is almost surely a function of \( Z \) conditional on \( X \). \( \square \)

12. Preparation for the proof of Theorem 5.1

In this section we prove a two lemmas that are needed for the proof of Theorem 5.1. Let \( Y \) be a random variable and \( X \) be an \( \mathbb{R}^p \)-valued random vector with bounded support, defined on the same probability space as \( Y \). Let \( X_1, \ldots, X_n \) be i.i.d. copies of \( X \). For each \( i \), let \( X_{n,i} \) be the nearest neighbor of \( X_i \), ties broken at random.

**Lemma 12.1.** Then there is a constant \( C \) depending only on the diameter of the support of \( X \) and the dimension \( p \), such that
\[
\mathbb{E}\|X_1 - X_{n,1}\| \leq \begin{cases} 
Cn^{-1} \log n & \text{if } p = 1, \\
Cn^{-1/p} & \text{if } p \geq 2.
\end{cases}
\]

**Proof.** Throughout the proof, \( C \) will denote any constant that depends only on the diameter of the support and the dimension. The value of \( C \) may change from line to line.

Take any \( t > 0 \). Notice that
\[
\mathbb{P}(\|X_1 - X_{n,1}\| \geq t) = \frac{1}{n} \mathbb{E}\{|i : \|X_i - X_{n,i}\| \geq t|\}.
\]

Since the support is bounded, there can be at most \( C t^{-p} \) points in the support such that the distance between any two is \( \geq t \). But the set of all
$X_i$ such that $\|X_i - X_{n,i}\| \geq t$ is clearly such a set. This shows that
\[
\mathbb{P}(\|X_1 - X_{n,1}\| \geq t) \leq \frac{C}{nt^p}.
\]
But the probability is also bounded by 1. Integrating the minimum of the two bounds as $t$ ranges from 0 to the diameter of the support gives the required bound. \hfill \square

**Lemma 12.2.** Let $Q = Q(Y, X)$ be defined as in equation (9.1) and $Q_n = Q_n(Y, X)$ be defined as in equation (7.3). Suppose that there is a constant $L$ such that for any $x, x' \in \mathbb{R}^p$ and any $t \in \mathbb{R},$
\[
|\mathbb{P}(Y \leq t \mid X = x) - \mathbb{P}(Y \leq t \mid X = x')| \leq L \|x - x'\|.
\]
Then there are positive constants $C_1, C_2$ and $C_3$ depending only the diameter of the support, the number $L$, and the dimension $p$, such that for any $t \geq 0,$
\[
\mathbb{P}(\|Q_n - Q\| \geq C_1 n^{-\min(1/p, 1/2)} + t) \leq C_2 e^{-C_3 n t^2}.
\]

**Proof.** Let $Q_n'$ and $\Delta_n$ be as in the proof of Lemma 9.8. By the Dvoretzky–Kiefer–Wolfowitz inequality [20, 38], we know that for any $x \geq 0,$
\[
\mathbb{P}(\sqrt{n} \Delta_n \geq x) \leq 2 e^{-2x^2}.
\]
From this it follows that $\mathbb{E}(\Delta_n) \leq n^{-1/2}$, and therefore by (9.2),
\[
\mathbb{E}|Q_n' - Q_n| \leq 3n^{-1/2}.
\]
Arguing as in the proof of Lemma 9.8, we get
\[
\mathbb{E}(Q_n') = \int (\mathbb{E}(G_{X_1}(t)G_{X_{n,1}}(t)) - G(t)^2) d\mu(t).
\]
On the other hand,
\[
Q = \int (\mathbb{E}(G_X(t)^2) - G(t)^2) d\mu(t).
\]
Since $G_X(t) \in [0, 1]$ for all $x$ and $t$, this gives
\[
|\mathbb{E}(Q_n') - Q| \leq \int |\mathbb{E}|G_{X_1}(t) - G_{X_{n,1}}(t)|| d\mu(t).
\]
Therefore, by (12.1),
\[
|\mathbb{E}(Q_n') - Q| \leq L \mathbb{E}\|X_1 - X_{n,1}\|,\]
and so by Lemma 12.1 and the inequality (12.2), we get
\[
|\mathbb{E}(Q_n) - Q| \leq \begin{cases} C n^{-1} \log n & \text{if } p = 1, \\ C n^{-1/p} & \text{if } p \geq 2, \end{cases}
\]
where $C$ depends only on the diameter of the support of $X$, the number $L$, and the dimension $p$. The desired result now follows by Lemma 9.9. \hfill \square
13. Proof of Theorem 5.1

Let \( j_1, j_2, \ldots, j_p \) be the complete ordering of all variables produced by the stepwise algorithm in FOCI. Let \( S_0 := \emptyset \), and for each \( 1 \leq k \leq p \), let \( S_k := \{ j_1, \ldots, j_k \} \). For \( k > p \), let \( S_k := S_p \). For any subset \( S \), let \( Q(Y, X_S) \) be defined as in (9.1) and let \( Q_n(Y, X_S) \) be defined as in (7.3). Notice that \( Q(Y, X_S) \) is the same as the quantity \( Q(S) \) defined in (5.1). Define these quantities to be zero if \( S = \emptyset \). Let \( K \) be the integer part of \( 1/\delta + 2 \). Let \( E' \) be the event that \(|Q_n(Y, X_{S_k}) - Q(Y, X_{S_k})| \leq \delta/8\) for all \( 1 \leq k \leq K \), and let \( E \) be the event that \( S_K \) is sufficient.

**Lemma 13.1.** Suppose that \( E' \) has happened, and also that

\[
Q_n(Y, X_{S_k}) - Q_n(Y, X_{S_{k-1}}) \leq \frac{\delta}{2}
\]

for some \( 1 \leq k \leq K \). Then \( S_{k-1} \) is sufficient.

**Proof.** If \( K > p \), there is nothing to prove. So let us assume that \( K \leq p \). Take any \( k \leq K \) such that (13.1) holds. An examination of the formula for \( T_n \) shows that for each \( k \), \( j_k \) is the index \( j \) that maximizes \( Q_n(Y, X_{S_{k-1} \cup \{j\}}) \) among all \( j \notin S_{k-1} \). Since \( E' \) has happened, this implies that for any \( j \notin S_{k-1} \),

\[
Q(Y, X_{S_{k-1} \cup \{j\}}) - Q(Y, X_{S_{k-1}}) \leq Q_n(Y, X_{S_{k-1} \cup \{j\}}) - Q_n(Y, X_{S_{k-1}}) + \frac{\delta}{4}
\]

\[
\leq Q_n(Y, X_{S_k}) - Q_n(Y, X_{S_{k-1}}) + \frac{\delta}{4}
\]

\[
\leq \frac{3\delta}{4}.
\]

Therefore since \( \delta > 0 \), the definition of \( \delta \) implies that \( S_{k-1} \) must be a sufficient subset of predictors. \( \square \)

**Lemma 13.2.** The event \( E' \) implies \( E \).

**Proof.** Suppose that \( E' \) has happened. Suppose also that (13.1) is violated for every \( 1 \leq k \leq K \). Since \( E' \) has happened, this implies that for each \( k \leq K \),

\[
Q(Y, X_{S_k}) - Q(Y, X_{S_{k-1}}) \geq Q_n(Y, X_{S_k}) - Q_n(Y, X_{S_{k-1}}) - \frac{\delta}{4}
\]

\[
\geq \frac{\delta}{4}.
\]

This gives

\[
Q(Y, X_{S_K}) = \sum_{k=1}^{K}(Q(Y, X_{S_k}) - Q(Y, X_{S_{k-1}}))
\]

\[
\geq K \frac{\delta}{4} \geq \left( \frac{1}{\delta} + 1 \right) \frac{\delta}{4} > \frac{1}{4}.
\]
But the variance of any \([0, 1]\)-valued random variable is bounded by \(1/4\), which implies that \(1/4\) is the maximum possible value of the statistic \(Q\). This yields a contradiction, proving that (13.1) must hold for some \(k \leq K\). Therefore by Lemma [13.1] \(S_K\) is sufficient.

**Lemma 13.3.** There are positive constants \(C_1, C_2\) and \(C_3\) depending only on \(\delta, B\) and \(L\), such that
\[
P(E'') \geq 1 - C_1p^2e^{-C_3n}.
\]

*Proof.* By assumptions (A1) and (A2), and Lemma [12.2], there are positive constants \(C_1, C_2\) and \(C_3\) depending only on \(B, L\) and \(K\), such that for any \(S\) of size \(\leq K\) and any \(t \geq 0\),
\[
P(|Q_n(Y, X_S) - Q(Y, X_S)| \geq C_1n^{-\min\{1/K,1/2\}} + t) \leq C_2e^{-C_3nt^2}.
\]

Call the event on the left \(A_{S,t}\). Let
\[
A_t := \bigcup_{|S| \leq K} A_{S,t}.
\]

Then by a simple union bound,
\[
P(A_t) \leq C_2p^K e^{-C_3nt^2}.
\]

Now choose \(t = \delta/16\). If \(n\) is so large that
\[
C_1n^{-\min\{1/K,1/2\}} \leq \frac{\delta}{16}, \tag{13.2}
\]
then the above bound implies that
\[
P(E') \geq 1 - C_2p^Ke^{-C_3n}, \tag{13.3}
\]
where \(C_3\) is some positive constant depending only on \(B, L\) and \(\delta\). Now, the condition (13.2) can be written as \(n \geq n_0\), where \(n_0\) depends only on \(B, L\) and \(\delta\). Choose a constant \(C_5 \geq C_2\) so large (again, depending only on \(B, L\) and \(\delta\)), that for any \(n < n_0\),
\[
C_5p^Ke^{-C_3n} \geq 1.
\]

Then if \(n < n_0\), we have \(P(E') \geq 1 - C_5p^Ke^{-C_3n}\). Combining with (13.3), we see that this inequality holds without any constraint on \(n\). □

**Lemma 13.4.** The event \(E'\) implies that \(\hat{S}\) is sufficient.

*Proof.* Suppose that \(E'\) has happened. Consider two cases. First, suppose that FOCI has stopped at step \(K\) or later. Then \(S_K \subseteq \hat{S}\). By Lemma [13.2] \(E\) has also happened, and hence \(S_K\) is sufficient. Therefore in this case, \(S\) is sufficient. Next, suppose that FOCI has stopped at step \(k-1 < K\). Then by the definition of the stopping rule, we see that
\[
Q_n(Y, X_{S_k}) \leq Q_n(Y, X_{S_{k-1}}).
\]

In particular, (13.1) holds. Since \(E'\) has happened, Lemma [13.1] now implies that \(\hat{S} = S_{k-1}\) is sufficient. □
It is clear that Lemmas 13.3 and 13.4 together imply Theorem 5.1.

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