ESTIMATING LARGE CAUSAL POLYTREE SKELETONS FROM SMALL SAMPLES

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ABSTRACT. We consider the problem of estimating the skeleton of a large causal polytree from a relatively small i.i.d. sample. This is motivated by the problem of determining causal structure when the number of variables is very large compared to the sample size, such as in gene regulatory networks. We give an algorithm that recovers the tree with high accuracy in such settings. The algorithm works under essentially no distributional or modeling assumptions other than some mild non-degeneracy conditions.

1. INTRODUCTION

Let $X = (X_i)_{i \in V}$ be a finite collection of random variables. Let $T$ be a tree with vertex set $V$. We will say that $T$ is a ‘causal polytree skeleton’ for $X$ if for any distinct $i, j, k \in V$ such that $j$ is on the path connecting $i$ and $k$ in $T$, at least one of the following two criteria hold:

- $X_i$ and $X_k$ are conditionally independent given $X_j$, or
- $X_i$ and $X_k$ are unconditionally independent.

(See Section 5 for the standard definition of a causal polytree skeleton and why the above definition is a generalization of that.) Let $p := |V|$ denote the number of variables. Let $X^1, \ldots, X^n$ be i.i.d. copies of $X$, which is the data we observe. Our goal is to estimate $T$ using this data. The main contribution of this article is an algorithm that can accurately estimate $T$ using $X^1, \ldots, X^n$ when $n \gg \log p$, under very mild conditions on the random variables. The algorithm is fully nonparametric, and works for discrete as well as continuous data. It is also quite fast, and works well on large datasets.

We give two kinds of evidence for our claims. First, we give a theoretical result with a finite sample error bound which gives a mathematical proof of the claim from the previous paragraph. Second, we give simulated examples where the algorithm performs well. For example, we have an example where $p = 1023$ and $n = 100$, and the algorithms recovers the correct edges with 93% accuracy. We avoid giving a real data example because in real data, it is not clear what the ‘real tree’ is, and therefore it is impossible to validate any claim of accurate reconstruction.

To put this work in its proper context, let us now discuss some of the relevant literature. The problem of estimating causal polytrees arises prominently in causal inference. One of the earliest attempts at reconstructing causal structures from data, under the assumption that the underlying graph is a tree, was due to Rebane and Pearl [27], who repurposed an old algorithm of Chow and Liu [8] to give a method for consistent estimation of causal polytrees (a term that was coined in [27]). It will be explained in Section 5 why causal polytrees, as defined in [27], are special cases of the causal polytrees defined above — but with a directional structure, whereas our trees

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are undirected. In the language of causal inference, we are trying to estimate the undirected ‘skeleton’ of the polytree.

The Rebane–Pearl approach has several drawbacks in the modern context. First, it is based on mutual information, just like the original Chow–Liu algorithm. Estimating mutual information from data is notoriously time-consuming (see [6] for some numbers), and moreover, requires special assumptions on the distribution of the data. Second, it is not clear if the algorithm works in modern problems where the number of variables is far greater than the sample size. Such examples arise routinely in gene regulatory networks, where we may have $n$ as small as a few hundred and $p$ as large as many thousands (see [31] for some examples).

The same problems persist in other popular classical algorithms for causal structure recovery (that go beyond trees), such as the PC algorithm [32] and the IC algorithm [24]. In the last two decades, several attempts have been made to design algorithms that work when the sample size is relatively small compared to the number of variables. For example, variants of the PC algorithm were shown to work when the number of variables grows polynomially with sample size [9, 18, 20]. These works are limited by the assumption that the variables are jointly Gaussian. A generalization to the case where the joint distribution is transformable to Gaussian using copulas was proposed in [14].

The above algorithms all use conditional independence testing of some form. Due to the well-known difficulties of conditional independence testing in the absence of stringent distributional assumptions [29], there is a different body of work that uses ‘score-based methods’ that do not need conditional independence testing. Score-based methods in the Gaussian setting have been proposed in [7, 19, 34]. The problem becomes less tractable in the absence of Gaussianity; solutions under various other structural assumptions have been proposed by various authors — see, e.g., [5, 16, 23, 25, 26, 30]. Methods that combine score-based methods with conditional independence testing have also been proposed, e.g., in [22, 33].

Although score-based algorithms avoid conditional independence testing, they have their own problems. For example, score-based algorithms are computationally rather expensive, to the extent that it is hard to use them when the number of variables is very large. (For some ideas about speeding up the calculations, see [4, 35].) Moreover, they often require strong assumptions on the distribution of the data.

To summarize the discussion, there is now a multitude of different algorithms for causal structure recovery, but they all suffer from at least one of the following problems: (a) They are not fully nonparametric, often requiring strong distributional or modeling assumptions. (b) They are computationally expensive and consequently hard to implement if the number of variables is large. (c) It is not clear — neither theoretically nor practically — if they truly work well when the number of variables is large compared to the sample size, even if the computational issue can be tackled.

Very recently, researchers have started paying attention to the above deficiencies of the algorithms proposed in the literature. Fully nonparametric methods have been proposed in [2, 11, 12] with finite sample guarantees. However, in spite of the finite sample guarantees, it is not clear if the methods proposed in these papers actually work well when the number of variables is much larger than the sample size. The same question arises in other recent works that specifically target large models, such as [17]. For example, in the simulated examples from [12, 17], $p$ is typically $\leq 100$, and $n$ is typically between 50 and 500. In the simulated examples from [2, 11], $n$ is taken to be of the order of several thousands, and $p$ less than 100.
In the light of the above discussion, we are now better poised to explain the main contribution of this paper. We have an algorithm that accurately recovers a causal polytree skeleton from the data even if the number of variables is much larger than the sample size. We require essentially no distributional or modeling assumptions, which makes our algorithm fully nonparametric. The efficacy of the algorithm is demonstrated through theoretical results and through concrete numerical examples where the number of variables is much larger than the sample size. The main deficiency of our approach is that it is applicable only when the causal structure is a tree. Another issue is that we make no effort to understand the directionality of the edges; our algorithm outputs a tree with undirected edges (the ‘DAG skeleton’, in the language of causal inference).

The paper is organized as follows. We present our algorithm in Section 2. The main theorem, which is the theoretical guarantee for our algorithm, is presented in Section 3. Simulated examples are in Section 4. In Section 5 we show that our definition of a causal polytree skeleton is a generalization of the standard definition. The main theorem is proved in Section 6.

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2. The Algorithm

Our algorithm makes use of a coefficient of correlation proposed recently in [6]. This is defined as follows. Let \((x_1, y_1), \ldots, (x_n, y_n)\) be \(n\) pairs of real numbers, where \(n \geq 2\). Let \(\pi\) be a permutation of \(1, \ldots, n\) such that \(x_{\pi(1)} \leq x_{\pi(2)} \leq \cdots \leq x_{\pi(n)}\). If there is more than one such permutation, choose one uniformly at random. For each \(i\), let \(r_i\) be the number of \(j\) such that \(y_j \leq y_{\pi(i)}\) and let \(l_i\) be the number of \(j\) such that \(y_j \geq y_{\pi(i)}\). Then define the \(\xi\)-coefficient between the \(x_i\)’s and the \(y_i\)’s as

\[
\xi_n := 1 - \frac{n \sum_{i=1}^{n-1} |r_{i+1} - r_i|}{2 \sum_{i=1}^{n} l_i(n - l_i)}.
\]  

(2.1)

Note that the \(\xi\)-coefficient is not symmetric — that is, the \(\xi\)-coefficient between the \(y_i\)’s and the \(x_i\)’s is not the same as the \(\xi\)-coefficient between the \(x_i\)’s and the \(y_i\)’s. Another thing to note is that the denominator on the right side is equal to zero if and only if all the \(y_i\)’s are equal. In this case, \(\xi_n\) is left undefined in [6]; but in this paper we define \(\xi_n\) to be 0 if this happens.

Let us now recall the setting introduced in Section 1. We have a finite collection of random variables \(X = (X_i)_{i \in V}\), and an undirected tree \(T\) that spans the vertex set \(V\). The tree \(T\) is a causal polytree skeleton for \(X\), meaning that if \(i, j, k \in V\) are distinct vertices such that \(j\) is on the path connecting \(i\) and \(k\) in \(T\), then either \(X_i\) and \(X_k\) are conditionally independent given \(X_j\) or \(X_i\) and \(X_k\) are unconditionally independent. Our data consists of \(n\) i.i.d. copies \(X^1, \ldots, X^n\) of the collection \(X\). We produce an estimate \(\hat{T}_n\) of \(T\) in the following two steps:

Step 1. Let \(X_i^m\) denote the \(i\)th coordinate of \(X^m\). For each distinct \(i, j \in V\), let \(\xi^m_{ij}\) denote the \(\xi\)-coefficient between \((X_i^m)_{1 \leq m \leq n}\) and \((X_j^m)_{1 \leq m \leq n}\). Define a subgraph \(G_n\) of the complete graph on \(V\) as follows. For each distinct pair of vertices \(i, j \in V\), keep the undirected edge \((i, j)\) in \(G_n\) if and only if there does not exist \(k \in V \setminus \{i, j\}\) such that

\[
\xi_{ki}^n \geq \xi_{ij}^n \quad \text{and} \quad \xi_{kj}^n \geq \xi_{ij}^n.
\]  

(2.2)
Step 2. For each undirected edge \((i, j)\) in \(G_n\), let \(w_{ij}^n := \min\{\xi_{ij}^n, \xi_{ji}^n\}\) be the weight of \((i, j)\). Let \(T_n\) be the maximal weighted spanning forest (MWSF) of \(G_n\) with these edge-weights. That is, \(T_n\) maximizes the sum of edge-weights among all spanning forests of \(G_n\). If there is more than one MWSF, choose one according to some arbitrary rule. This \(T_n\) is our estimate of \(T\).

The first step of the above algorithm is inspired by a proposal from [31], where a coefficient called the ‘φ-mixing coefficient’ [1] is used with similar intent, instead of the \(\xi\)-coefficient. The second step is inspired by the Chow–Liu algorithm [8] mentioned earlier, with mutual information replaced by the \(w\)-weights defined above.

3. Theoretical Guarantee

To state our theoretical guarantee for the algorithm introduced in the previous section, we need a small amount of preparation. First, recall that the maximal correlation coefficient \(R(X, Y)\) between two random variables \(X\) and \(Y\) [13, 28] is defined as the supremum of the Pearson correlation between \(f(X)\) and \(g(Y)\) over all measurable functions \(f\) and \(g\) such that \(f(X)\) and \(g(Y)\) have finite and nonzero variance. It is easy to see that \(R(X, Y) \in [0, 1]\). Note that if \(X\) is a constant, then there will not exist an \(f\) as above. In this case, we define \(R(X, Y) = 0\). Similarly, we let \(R(X, Y) = 0\) if \(Y\) is a constant.

Next, for a random variable \(X\), we define a quantity \(\alpha(X)\) that measures the ‘degree to which \(X\) is not a constant’, as \(\alpha(X) := P(X \neq X')\) where \(X'\) is an independent copy of \(X\). We will refer to it as the ‘\(\alpha\)-coefficient’ of \(X\). Note that \(\alpha(X) > 0\) if and only if \(X\) is not a constant.

Lastly, recall that if \((X_1, Y_1), (X_2, Y_2), \ldots\) are i.i.d. copies of a pair of random variables \((X, Y)\), where \(Y\) is non-constant, and \(\xi_n\) is the \(\xi\)-correlation coefficient between \(X_1, \ldots, X_n\) and \(Y_1, \ldots, Y_n\), then one of the main results of [6] is that as \(n \to \infty\), \(\xi_n\) converges in probability to the limit

\[
\xi(X, Y) = \frac{\int \text{Var}(E(1_{\{Y \geq t\}}|X))d\mu(t)}{\int \text{Var}(1_{\{Y \geq t\}})d\mu(t)}
\]

(3.1)

where \(\mu\) is the law of \(Y\). Moreover, \(\xi(X, Y)\) is always in \([0, 1]\), \(\xi(X, Y) = 0\) if and only if \(X\) and \(Y\) are independent, and \(\xi(X, Y) = 1\) if and only if \(Y\) is equal to a measurable function of \(X\) with probability one. The only assumption required for this result is that \(Y\) is not a constant. We will refer to \(\xi(X, Y)\) as the ‘\(\xi\)-correlation’ between \(X\) and \(Y\). In this article, we will prove the auxiliary result that \(E(\xi_n)\) converges to \(\xi(X, Y)\) as \(n \to \infty\). This does not directly follow from the results of [6]; a small additional argument is needed (see Corollary 6.2). In [6], \(\xi(X, Y)\) is left undefined if \(Y\) is a constant; in this article, we define \(\xi(X, Y)\) to be 0 if \(Y\) is a constant.

Let us now return to the setting of Section 2. The following theorem shows, in essence, that \(T_n = T\) with high probability if no \(X_i\) is a constant, no \(X_i\) and \(X_j\) are independent when \(i\) and \(j\) are neighbors in \(T\), no \(X_i\) and \(X_j\) have maximal correlation 1 when \(i\) and \(j\) are neighbors in \(T\), and \(n \gg \log p\).

**Theorem 3.1.** Let \(X = (X_i)_{i \in V}\) be a finite collection of random variables with a causal polytree skeleton \(T\), as defined at the beginning of Section 1 and let \(p := |V|\). Let \(T_n\) be the estimate of \(T\) based on a sample of \(n\) i.i.d. copies of \(X\), as defined in Section 2. For each \(i\) and \(j\), let \(\xi_{ij}\) be the \(\xi\)-correlation coefficient between \(X_i\) and \(X_j\), let \(R_{ij}\) be the maximal correlation coefficient between \(X_i\) and \(X_j\), and let \(\alpha_i\) be the \(\alpha\)-coefficient of \(X_i\), as defined above. Suppose that there is a positive constant \(\delta\) such that
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(1) $\xi_{ij} \geq \delta$ whenever $(i, j)$ is an edge in $T$,
(2) $R_{ij} \leq 1 - \delta$ whenever $(i, j)$ is an edge in $T$, and
(3) $\alpha_i \geq \delta$ for all $i \in V$.

Furthermore, suppose that $n$ is so large that $|\mathbb{E}(\xi_{ij}^n) - \xi_{ij}| \leq \delta^2/8$ for all distinct $i, j \in V$. Then there exist positive constants $C_1(\delta)$ and $C_2(\delta)$ depending only on $\delta$, such that

$$\mathbb{P}(T_n \neq T) \leq C_1(\delta)p^2 e^{-C_2(\delta)n}.$$ 

In particular, if $R_{ij} < 1$ and $X_i$ and $X_j$ are dependent for all edges $(i, j)$ in $T$, and each $X_i$ is non-constant, then $\mathbb{P}(T_n \neq T) \to 0$ as $n \to \infty$.

We remark that the lower bound on $n$ required in the above result is likely to depend only on $\delta$ in non-pathological situations, because it depends only on the joint distributions on $(X_i, X_j)$ over all edges $(i, j)$ in $T$. If none of these joint distributions are too ‘weird’, the condition $|\mathbb{E}(\xi_{ij}^n) - \xi_{ij}| \leq \delta^2/8$ is likely to be satisfied for all $n$ exceeding some threshold depending only on $\delta$.

Another small remark is that the theorem shows that if for all edges $(i, j)$ in $T$, $R_{ij} < 1$ and $X_i$ and $X_j$ are dependent, and each $X_i$ is non-constant, then $T$ must be the unique causal polytree skeleton.

4. SIMULATED EXAMPLES

In this section, we present simulation results for four kinds of trees. The code used for all of the following is available at [https://souravchatterjee.su.domains/condep.R](https://souravchatterjee.su.domains/condep.R).

The first is the linear tree, which is a sequence of nodes arranged in a line, with adjacent ones joined by edges. If there are $p$ nodes, the random variables $X_1, \ldots, X_p$ are generated according to the recursion

$$X_i = \frac{X_{i-1} + \epsilon_i}{\sqrt{2}}$$

with $X_1 = \epsilon_1$, where $\epsilon_1, \ldots, \epsilon_p$ are i.i.d. $N(0, 1)$ random variables.

The second is the binary tree, which has a root node with two children, each child has two children of its own, and so on. If $p$ is the number of nodes, we denote them by $1, \ldots, p$, with 1 denoting the root node. If $i$ is the parent of a node $j$, we define

$$X_j = \frac{X_i + \epsilon_j}{\sqrt{2}},$$

with $X_1 = \epsilon_1$, where again $\epsilon_1, \ldots, \epsilon_p$ are i.i.d. $N(0, 1)$ random variables.

The third is the star tree, which has one central node and the other nodes are all children of the central node. If the nodes are marked $1, \ldots, p$, we let 1 be the central node. We let $X_1 = \epsilon_1$, and for each $i \geq 2$, we let

$$X_i = \frac{X_1 + \epsilon_i}{\sqrt{2}},$$

where $\epsilon_1, \ldots, \epsilon_p$ are i.i.d. $N(0, 1)$ random variables.

Finally, the fourth is the reverse binary tree, which is exactly the same as the binary tree, but the random variables are defined differently. Here, we let $X_1$ to be an independent $N(0, 1)$
random variable for each leaf $i$. Then, we define the $X_i$’s for the remaining nodes by backward induction as follows. If $i$ is an internal node with children $j$ and $k$, we define

$$X_i = \frac{X_j + X_k + \epsilon_i}{\sqrt{3}},$$

where $\epsilon_i$’s are i.i.d. $N(0, 1)$ random variables. It is not hard to see that the trees described in each of the above examples are indeed causal polytree skeletons of the $X_i$’s.

For each of these models, we try out our algorithm with various values of $n$ and $p$. The accuracy of the output is measured by the proportion of edges that are correctly identified. Since any spanning tree has $p - 1$ edges, this is a reasonable measure of discrepancy. The average value of this proportion in 20 simulations is then calculated for each case. The results are tabulated in Table 1. Since $p$ must be of the form $2^k - 1$ for the binary tree example, we take all our $p$’s of this form. To be specific, we take $p = 15$, $p = 511$ and $p = 1023$, and for each $p$, we consider $n = 50$, $n = 100$, $n = 200$ and $n = 300$.

From Table 1 we see that for the linear tree and the binary tree, our algorithm performs very well (more than 90% edges correctly recovered) even for $n = 100$ and $p = 1023$. The star tree and the reverse binary tree are harder to estimate, with the reverse binary tree requiring $n = 200$ for a recovery rate greater than 90% (for $p = 1023$), and the star tree requiring $n = 300$.

5. STANDARD DEFINITION OF A CAUSAL POLYTREE

Let $X = (X_i)_{i \in V}$ be a finite collection of random variables. Let $G$ be a directed acyclic graph (DAG) with vertex set $V$. For each $i \in V$, let $p(i)$ denote the set of ‘parents’ of $i$ in $G$, that is, the set of nodes with arrows pointing towards $i$. We say that dependency structure of $X$ is described by the DAG $G$ if the joint density of $X$ (with respect to some product measure) can be factorized as

$$f(x) = \prod_{i \in V} f_i(x_i | (x_j)_{j \in p(i)}),$$

(5.1)
where \( f_i \) is the conditional density of \( X_i \) given its parents. If \( p(i) \) is empty, \( f_i \) is the unconditional density of \( X_i \). The ‘skeleton’ of the DAG \( G \) is the undirected graph obtained by forgetting the directionailities of the edges. If the skeleton is a tree, we say that \( G \) is a causal polytree.

The following result shows that our definition of a causal polytree skeleton in Section 1 is a generalization of the standard definition.

**Proposition 5.1.** A causal polytree skeleton, as defined above, is also a causal polytree skeleton in the sense defined in Section 1.

**Proof.** Let \( T \) be the skeleton of a causal polytree skeleton for a collection \( X = (X_i)_{i \in V} \), as defined above. Let the function \( f \) displayed in equation (5.1) be the joint probability density of \( X \) with respect to some product measure. Take any distinct \( i, j, k \in V \) such that \( j \) lies on the path connecting \( i \) and \( k \) in \( T \).

For each \( a \in V \setminus \{j\} \), let \( q(a) \) be the unique neighbor of \( j \) which belongs to the path connecting \( a \) and \( j \) in \( T \). Let \( b_1, \ldots, b_m \) be the parents of \( j \) (where \( m \) may be 0), and for each \( 1 \leq l \leq m \), let \( V_l \) be the set of all \( a \) such that \( q(a) = b_l \). Let \( V_0 \) be the set of all \( a \) such that \( q(a) \) is not a parent of \( j \). Let \( U := V_1 \cup \ldots \cup V_m \).

Now note that in the product displayed in (5.1), \( x_a \) and \( x_b \) can be in the same factor only if either \( a \) is a parent of \( b \), or \( b \) is a parent of \( a \), and \( a \) and \( b \) have a common child. Thus, if \( a \in V_0 \) and \( b \in U \), then \( x_a \) and \( x_b \) cannot appear in a common factor. This shows that the collections \( (X_a)_{a \in V_0} \) and \( (X_b)_{b \in U} \) are conditionally independent given \( X_j \). In particular, if \( i \in V_0 \) and \( k \in U \), or if \( i \in U \) and \( k \in V_0 \), then \( X_i \) and \( X_k \) are conditionally independent given \( X_j \).

The only other possibility is that \( i \in V_l \) and \( k \in V_{l'} \) for some \( 1 \leq l \neq l' \leq m \). We will show that in this case, \( X_i \) and \( X_k \) are unconditionally independent. First, take any \( a \in V_0 \) which has no children. Then we can integrate out \( x_a \) in the product (5.1) and remove it from the graph. The resulting model is again described by a DAG whose skeleton is a forest, because we are simply removing a vertex and the edges incident to it.

Continuing like this, we can iteratively remove all vertices in \( V_0 \), leaving us with only \( U \cup \{j\} \). Integrating out \( x_j \), we now see that the collections \( (X_a)_{a \in V_0}, l = 1, \ldots, m \) are independent. This shows that \( X_i \) and \( X_k \) are independent. \( \square \)

### 6. Proof of Theorem 5.1

The proof of Theorem 5.1 requires several steps. These are divided into subsections below, for the reader’s convenience.

#### 6.1. Concentration of \( \xi_n \)

Let \( (X, Y) \) be a pair of real-valued random variables. Let \( n \geq 2 \) and let \((X_1, Y_1), \ldots, (X_n, Y_n)\) be i.i.d. copies of \((X, Y)\). Let \( \xi_n \) be the \( \alpha \)-coefficient between \( X_1, \ldots, X_n \) and \( Y_1, \ldots, Y_n \). Recall the \( \alpha \)-coefficient defined in Section 3. The goal of this subsection is to prove the following result.

**Proposition 6.1.** Suppose that \( \alpha(Y) \) is bounded below by some \( \delta > 0 \). Then, there are positive numbers \( C_1(\delta), C_2(\delta) \) and \( C_3(\delta) \) depending only on \( \delta \) such that for all \( t \in [0, C_1(\delta)] \) and all \( n \),

\[
\mathbb{P}(|\xi_n - \mathbb{E}(\xi_n)| \geq t) \leq C_2(\delta) e^{-C_3(\delta) n t^2}.
\]

This immediately yields the following corollary.

**Corollary 6.2.** If \( Y \) is not a constant, then as \( n \to \infty \), \( \mathbb{E}(\xi_n) \to \xi \), where \( \xi \) is the \( \xi \)-correlation between \( X \) and \( Y \) displayed in equation (5.1).
Proof. By [6, Theorem 1.1], $\xi_n \to \xi$ in probability as $n \to \infty$. By Proposition 6.1, $\xi_n - \mathbb{E}(\xi_n) \to 0$ in probability. The claim is proved by combining these observations. \(\square\)

To prove Proposition 6.1, we need two lemmas. The first one is the following.

**Lemma 6.3.** Let $\alpha := \alpha(Y)$ and let $\mu$ be the law of $Y$. For each $t \in \mathbb{R}$, let $G(t) := \mathbb{P}(Y \geq t)$.

Let

$$\beta := \int G(t)(1 - G(t))d\mu(t).$$

Then $\beta \geq \alpha^2/32$.

**Proof.** Let $Y'$ be an independent copy of $Y$. Then note that

$$\mathbb{P}(Y > Y') = \mathbb{P}(Y < Y'),$$

and thus,

$$\mathbb{P}(Y' \geq Y) = \frac{1}{2}(\mathbb{P}(Y' > Y) + \mathbb{P}(Y' < Y)) = \frac{1}{2}(1 - \mathbb{P}(Y' = Y)).$$

This gives

$$\mathbb{P}(Y' \geq Y) = \mathbb{P}(Y' > Y) + \mathbb{P}(Y' = Y) = \frac{1}{2}(1 + \mathbb{P}(Y' = Y)) = 1 - \frac{\alpha}{2}.$$

But $\mathbb{P}(Y' \geq Y) = \mathbb{E}(G(Y))$. Thus,

$$\int G(t)d\mu(t) = 1 - \frac{\alpha}{2} \quad (6.1)$$

Take any $\epsilon \in (0, 1/2)$. Define three sets

$$A_\epsilon := \{t : G(t) > 1 - \epsilon\}, \quad B_\epsilon := \{t : \epsilon \leq G(t) \leq 1 - \epsilon\}, \quad C_\epsilon := \{t : G(t) < \epsilon\}.$$

Then

$$\int G(t)d\mu(t) \geq (1 - \epsilon)\mu(A_\epsilon).$$

Combining this with (6.1), we get

$$\mu(A_\epsilon) \leq \frac{1}{1 - \epsilon} \left(1 - \frac{\alpha}{2}\right).$$

On the other hand, since $G$ is a non-increasing left-continuous function, the set $C_\epsilon$ is an interval of the form $(t, \infty)$. Thus,

$$\mu(C_\epsilon) = \mu((t, \infty)) = \lim_{s \downarrow t} G(s) \leq \epsilon.$$

Combining the last two displays, we get

$$\mu(B_\epsilon) = 1 - \mu(A_\epsilon) - \mu(B_\epsilon) \geq 1 - \frac{1}{1 - \epsilon} \left(1 - \frac{\alpha}{2}\right) - \epsilon.$$
But \( G(t)(1 - G(t)) \geq \epsilon(1 - \epsilon) \) on \( B_\epsilon \) since \( \epsilon \in (0, 1/2) \). Thus,
\[
\beta \geq \epsilon(1 - \epsilon) \mu(B_\epsilon) \\
\geq \epsilon(1 - \epsilon) - \epsilon \left(1 - \frac{\alpha}{2}\right) - \epsilon^2(1 - \epsilon) \\
= \frac{\epsilon \alpha}{2} - 2\epsilon^2 + \epsilon^3 \geq \frac{\epsilon \alpha}{2} - 2\epsilon^2.
\]
Choosing \( \epsilon = \alpha/8 \) completes the proof. \( \square \)

The second lemma we need is the following simple upper bound on \( \xi_n \).

**Lemma 6.4.** For any \( n \) and any realization of the data, \( |\xi_n| \leq 1 + n^2 \).

**Proof.** If \( Y_1 = Y_2 = \cdots = Y_n \) in a particular realization of the data, then \( \xi_n = 0 \) by the convention introduced in Section 2. So, let us assume that not all the \( Y_i \)'s are equal. Recall the \( r_i \)'s and \( l_i \)'s used in the definition of \( \xi_n \) in Section 2. Since the \( Y_i \)'s are not all equal, it is easy to see that there is at least one \( l_i \) which lies strictly between 0 and \( n \). Thus, for this \( i \), \( l_i(n - l_i) \geq n \).

Since \(|r_{i+1} - r_i| \leq n\) for each \( i \), inspecting the formula (2.1) now shows that
\[
|\xi_n| \leq 1 + n^2.
\]

We are now ready to prove Proposition 6.1.

**Proof of Proposition 6.1.** Define
\[
G_n(t) := \frac{1}{n} \sum_{i=1}^{n} 1(Y_i \geq t).
\]
Define
\[
S_n := \frac{1}{n} \sum_{i=1}^{n} G_n(Y_i)(1 - G_n(Y_i)), \quad S'_n := \frac{1}{n} \sum_{i=1}^{n} G(Y_i)(1 - G(Y_i)).
\]
Recall the number \( \beta \) defined in Lemma 6.3. Note that \( \mathbb{E}(S'_n) = \beta \) and \( S'_n \) is an average of i.i.d. random variables taking values in \([0, 1]\). Therefore, by Hoeffding’s inequality [15],
\[
P(|S'_n - \beta| \geq t) \leq 2e^{-2nt^2}
\]
for any \( t \geq 0 \). Let \( \Delta_n := \sup_{t \in \mathbb{R}} |G_n(t) - G(t)| \). By the Dvoretzky–Kiefer–Wolfowitz inequality [10, 21],
\[
P(\Delta_n \geq t) \leq 2e^{-2nt^2}
\]
for any \( t \geq 0 \). Now, by the triangle inequality, \( |S_n - S'_n| \leq 2\Delta_n \). Combining all of this, we get that for any \( t \geq 0 \),
\[
P(|S_n - \beta| \geq t) \leq P(|S_n - S'_n| \geq t/2) + P(|S'_n - \beta| \geq t/2) \leq P(\Delta_n \geq t/4) + P(|S'_n - \beta| \geq t/2) \leq 4e^{-nt^2/8}.
\]
From the proof of [6, Theorem 1.1] in the supplementary materials of [6], recall that
\[
\left| \frac{Q_n}{S_n} - \xi_n \right| \leq \frac{1}{2nS_n}, \quad (6.2)
\]
where \( Q_n \) is a random variable taking values in \([-1, 1]\), which has a somewhat complicated definition that is unnecessary to state here. The only thing we need to know about \( Q_n \) is that for all \( t \geq 0 \),
\[
\mathbb{P}(|Q_n - \mathbb{E}(Q_n)| \geq t) \leq 2e^{-Cn t^2},
\]
where \( C \) is a positive universal constant. Now, if \(|Q_n - \mathbb{E}(Q_n)| < t\) and \(|S_n - \beta| < t\) for some \( t \in [0, \beta/2] \), then \( S_n > \beta/2 \), and hence
\[
\left| \frac{Q_n - \mathbb{E}(Q_n)}{S_n} \right| = \frac{|Q_n - \mathbb{E}(Q_n)|}{S_n} \leq \frac{2}{\beta^2} |Q_n| \leq \frac{2}{\beta^2} \left( |Q_n| \mathbb{E}(Q_n) + \mathbb{E}(Q_n)|S_n - \beta| \right) \leq \frac{2(\beta + 1)t}{\beta^2},
\]
and consequently, by (6.2),
\[
\left| \frac{\xi_n - \mathbb{E}(Q_n)}{\beta} \right| \leq \frac{2(\beta + 1)t}{\beta^2} + \frac{1}{2nS_n} \leq \frac{2(\beta + 1)t}{\beta^2} + \frac{1}{n\beta}.
\]
Let \( a_n := \mathbb{E}(Q_n)/\beta \). From the above, we see that for all \( t \in [0, \beta/2] \),
\[
\mathbb{P}\left(|\xi_n - a_n| \geq \frac{2(\beta + 1)t}{\beta^2} + \frac{1}{n\beta}\right) \leq 6e^{-Cn t^2}
\]
where \( C \) is a positive universal constant. By Lemma 6.3 and Lemma 6.4, it is easy to see using the above inequality that
\[
|\mathbb{E}(\xi_n) - a_n| \leq \mathbb{E}|\xi_n - a_n| = \int_0^\infty \mathbb{P}(|\xi_n - a_n| \geq t) dt \leq \frac{C(\delta)}{\sqrt{n}},
\]
where \( C(\delta) \) is a positive constant that depends only on \( \delta \). Thus, again using (6.3), we get that there are positive numbers \( C_1(\delta) \), \( C_2(\delta) \) and \( C_3(\delta) \) depending only on \( \delta \) such that for all \( t \in [0, C_1(\delta)] \) and all \( n \),
\[
\mathbb{P}\left(|\xi_n - \mathbb{E}(\xi_n)| \geq t + \frac{C_2(\delta)}{\sqrt{n}}\right) \leq 6e^{-C_3(\delta)n t^2}.
\]
Now, if \( t \geq 2C_2(\delta)/\sqrt{n} \) and \( t \leq C_1(\delta) \), the above inequality implies that
\[
\mathbb{P}\left(|\xi_n - \mathbb{E}(\xi_n)| \geq t\right) \leq \mathbb{P}\left(|\xi_n - \mathbb{E}(\xi_n)| \geq \frac{t}{2} + \frac{C_2(\delta)}{\sqrt{n}}\right) \leq 6e^{-C_3(\delta)n t^2/4}.
\]
On the other hand, if \( t < 2C_2(\delta)/\sqrt{n} \), then
\[
\mathbb{P}\left(|\xi_n - \mathbb{E}(\xi_n)| \geq t\right) \leq 1 \leq e^{4C_3(\delta)C_2(\delta)^2} e^{-C_3(\delta)n t^2}.
\]
Combining the last two displays completes the proof. \( \square \)
6.2. **Data processing inequality for maximal correlation.** In this subsection we prove that the maximal correlation coefficient satisfies an inequality that is also satisfied by mutual information, going by the name ‘data processing inequality’.

**Proposition 6.5.** Let $X$, $Y$ and $Z$ be three random variables such that $Y$ and $Z$ are conditionally independent given $X$. Then $R(Z,Y) \leq R(X,Y)$.

**Proof.** If $Y$ is a constant or $Z$ is a constant, then $R(Z,Y) = 0$ by definition, and so there is nothing to prove. So, let us assume that both $Y$ and $Z$ are non-constant. In this case, if $X$ is a constant, then the conditional independence of $Y$ and $Z$ given $X$ implies that $Y$ and $Z$ are unconditionally independent, and hence $R(Z,Y) = 0$. So, again, there is nothing to prove. Thus, let us assume that $X$ is also non-constant.

Take any $f$ and $g$ such that $\text{Var}(f(Z))$ and $\text{Var}(g(Y))$ are both in $(0, \infty)$. Without loss of generality, $\mathbb{E}(f(Z)) = \mathbb{E}(g(Y)) = 0$ and $\text{Var}(f(Z)) = \text{Var}(g(Y)) = 1$. Then by the conditional independence of $Y$ and $Z$ given $X$, we have

$$\text{Corr}(f(Z), g(Y)) = \mathbb{E}(f(Z)g(Y)) = \mathbb{E}(h(X)g(Y)),$$

where $h(X) := \mathbb{E}(f(Z)|X)$. But $\mathbb{E}(h(X)) = \mathbb{E}(f(Z)) = 0$, and so

$$\mathbb{E}(h(X)g(Y)) \leq R(X,Y)\sqrt{\mathbb{E}(h(X)^2)\mathbb{E}(g(Y)^2)} = R(X,Y)\sqrt{\mathbb{E}(h(X)^2)}.$$

To complete the proof, note that $\mathbb{E}(h(X)^2) \leq \mathbb{E}(f(Z)^2) = 1$. \hfill $\square$

6.3. **Data processing inequality for $\xi$-correlation.** In this section we will show that the $\xi$-correlation also satisfies a data processing inequality, although it is a ‘one-sided’ version of the inequality, since the $\xi$-correlation is not symmetric. More importantly, the result makes a connection between the $\xi$-correlation and the maximal correlation, which will be important in the proof of Theorem 3.1.

**Proposition 6.6.** Let $X$, $Y$ and $Z$ be three random variables such that $Y$ and $Z$ are conditionally independent given $X$. Then $\xi(Z,Y) \leq R(Z,X)^2\xi(X,Y)$. In particular, $\xi(Z,Y) \leq \xi(X,Y)$.

**Proof.** If $Y$ is a constant, then both $\xi(Z,Y)$ and $\xi(X,Y)$ are zero (according to the convention adopted in Section 3), so there is nothing to prove. Thus, let us assume that $Y$ is not a constant. Take any $t \in \mathbb{R}$. Let $f(X) := \mathbb{P}(Y \geq t|X)$ and $g(Z) := \mathbb{P}(Y \geq t|Z)$. By the conditional independence of $Y$ and $Z$ given $X$, $g(Z) = \mathbb{E}(f(X)|Z)$. Let $\tilde{f}(X) := f(X) - \mathbb{E}(f(X))$ and $\tilde{g}(Z) := g(Z) - \mathbb{E}(g(Z))$. Since $\mathbb{E}(f(X)) = \mathbb{E}(g(Z))$, we have $\mathbb{E}(\tilde{f}(X)|Z) = \tilde{g}(Z)$. Thus,

$$\text{Var}(g(Z)) = \mathbb{E}(\tilde{g}(Z)^2)$$

$$= \mathbb{E}(\tilde{g}(Z)\tilde{f}(X)|Z))$$

$$= \mathbb{E}(\tilde{g}(Z)\tilde{f}(X)) \leq R(Z,X)\sqrt{\mathbb{E}(\tilde{g}(Z)^2)\mathbb{E}(\tilde{f}(X)^2)}.$$

Rearranging this inequality, we get

$$\text{Var}(g(Z)) \leq R(Z,X)^2\text{Var}(f(X)).$$
Since \( t \) is arbitrary, this implies that
\[
\xi(Z, Y) = \int \frac{\text{Var}(P(Y \geq t|Z))d\mu(t)}{\int \text{Var}(1_{Y \geq t})d\mu(t)} \\
\leq \int \frac{R(Z, X)^2\text{Var}(P(Y \geq t|X))d\mu(t)}{\int \text{Var}(1_{Y \geq t})d\mu(t)} = R(Z, X)^2\xi(X, Y),
\]
which completes the proof. \( \square \)

6.4. A fact about maximal spanning trees. The final bit of preliminary factoid that we need is the following result about maximal weighted spanning trees.

**Lemma 6.7.** Let \( T \) be a maximal weighted spanning tree of a connected weighted graph \( G = (V, E) \). If an edge \( e \) in \( G \) does not belong to \( T \), then every edge in the path connecting the endpoints of \( e \) in \( T \) must have weight greater than or equal to the weight of \( e \).

**Proof.** Suppose that some edge \( f \) in the path connecting the endpoints of \( e \) in \( T \) has \( w_f < w_e \). Then deleting \( f \) and adding \( e \) to \( T \) gives us a spanning tree whose weight is strictly greater than that of \( T \), which contradicts the maximality of \( T \). \( \square \)

This completes the preliminary steps. We are now ready to prove Theorem 3.1.

6.5. **Proof of Theorem 3.1.** First, take any distinct \( i, j \in V \). Let \( k \) be the vertex adjacent to \( j \) on the path joining \( i \) to \( j \) in \( T \). Then by Proposition 6.5 and the assumption that \( R_{kj} \leq 1 - \delta \) from the statement of Theorem 3.1, we get that \( R_{ij} \leq R_{kj} \leq 1 - \delta \). Thus,
\[
R_{ij} \leq 1 - \delta \quad \text{for all distinct} \quad i, j \in V.
\]

Take any distinct \( i, j, k \in V \) such that \( j \) is on the path connecting \( i \) and \( k \) in \( T \). Then either \( X_i \) and \( X_k \) are conditionally independent given \( X_j \), or \( X_i \) and \( X_k \) are unconditionally independent.

In the first case, by Proposition 6.6 and the inequality (6.4),
\[
\xi_{ki} \leq R_{kj}^2\xi_{ji} \leq (1 - \delta)^2\xi_{ji}. \tag{6.5}
\]

In the second case, \( \xi_{ki} = 0 \), and so the above inequality holds anyway. If \( i \) and \( j \) are neighbors, this shows that
\[
\xi_{ki} \leq \xi_{ji} - (2\delta - \delta^2)\xi_{ji} \leq \xi_{ji} - (2\delta - \delta^2)\delta, \tag{6.6}
\]
because \( 2\delta - \delta^2 > 0 \) and \( \xi_{ji} \geq \delta \). Define \( \gamma := (2\delta - \delta^2)\delta \). Note that since \( \delta > 0 \), \( 2\delta > \delta^2 \) and \( 2\delta - \delta^2 \leq 1 \) (because \( (1 - \delta)^2 \geq 0 \)), we have
\[
0 < \gamma \leq \delta. \tag{6.7}
\]

We claim that if in a particular realization of \( X^1, \ldots, X^n \), we have
\[
|\xi^n_{ij} - \xi_{ij}| \leq \frac{\gamma}{4} \quad \text{for all} \quad i, j, \tag{6.8}
\]
then \( T_n = T \). To see this, suppose that (6.8) holds in some realization of the data. First, taking any edge \( (i, j) \) in \( T \), let us show that \( (i, j) \) is in \( G_n \). Deleting the edge \( (i, j) \) from \( T \) splits \( T \) into two disjoint connected components \( A \) and \( B \), with \( i \in A \) and \( j \in B \). Take any \( k \in A \setminus \{i\} \).
Then by the definition of $\gamma$ and the inequality (6.6), we have $\xi_{ij} \geq \xi_{kj} + \gamma$. Thus, by (6.8) and (6.7),

$$\xi^n_{ij} \leq \xi_{kj} + \frac{\gamma}{4} \leq \xi_{ij} - \gamma + \frac{\gamma}{4} \leq \xi^n_{ij}$$

Similarly, if $k \in B \setminus \{j\}$, $\xi^n_{ki} < \xi^n_{ij}$. Therefore, for any $k \in V \setminus \{i, j\}$, the condition (2.2) is violated. This shows that $(i, j)$ is an edge in $G_n$.

Thus, $T$ is a subgraph of $G_n$ under (6.8). This shows, in particular, that $G_n$ is connected. Now recall that $T_n$ is an MWSF of $G_n$ when the edges are endowed with the weights $w^n_{ij}$. By (6.7) and the definition of $\delta$, we have

$$w_{ij} \geq \delta \geq \gamma > 0 \quad \text{for all edges} \quad (i, j) \in T.$$

Thus, under (6.8), by (6.7) we get

$$w^n_{ij} \geq \delta - \frac{\gamma}{4} > \frac{\delta}{2} > 0 \quad \text{for all edges} \quad (i, j) \in T. \quad (6.10)$$

Since $T_n$ is an MWSF of the connected graph $G_n$ and every edge-weight is strictly positive (by (6.10)), we deduce that $T_n$ is a maximal weighted spanning tree of $G_n$ under (6.8). Moreover, as noted above, $T$ is a spanning tree of $G_n$. Thus, to show that $T = T_n$, we only need to prove that any edge of $G_n$ that is not in $T$ cannot be in $T_n$.

So, take any edge $(i, j)$ of $G_n$ that is not in $T$ but is in $T_n$. We will prove by contradiction that such an edge cannot exist. First, we claim that $w^n_{ij} > \delta/2$. Let $P$ be the path in $T$ that connects $i$ to $j$. Then by (6.10), we have that $w^n_{kl} > \delta/2$ for every edge $(k, l)$ in $P$.

Since $(i, j)$ is an edge in $T_n$, deleting the edge $(i, j)$ splits $T_n$ into two components $A$ and $B$, with $i \in A$ and $j \in B$. Since $P$ connects $i$ to $j$ in $T$, there must be at least one edge $(k, l)$ in $P$ such that $k \in A$ and $l \in B$. Then note that $(k, l)$ is not an edge of $T_n$, and the path joining $k$ to $l$ in $T_n$ contains $(i, j)$. By Lemma 6.7 and the fact that $(i, j)$ is in $G_n$, this proves that $w^n_{ij} \geq w^n_{kl} > \delta/2$.

Next, to get a contradiction, we will show that $w^n_{ij} \leq \delta/2$. Take any vertex $k$ in $P$ that is not $i$ or $j$. Since $(i, j)$ is an edge of $G_n$, it follows that either $\xi^n_{ki} < \xi^n_{ij}$ or $\xi^n_{kj} < \xi^n_{ij}$. Suppose that $\xi^n_{ki} < \xi^n_{ij}$. Then by (6.8) and (6.5),

$$\xi^n_{ij} \leq \xi_{ij} + \frac{\gamma}{4} \leq (1 - \delta)^2 \xi_{ki} + \frac{\gamma}{4} \leq (1 - \delta)^2 \left( \xi^n_{ki} + \frac{\gamma}{4} \right) + \frac{\gamma}{4}$$

Rearranging this inequality, we get

$$\xi^n_{ij} \leq \frac{1}{2\delta - \delta^2} \left( (1 - \delta)^2 \frac{\gamma}{4} + \frac{\gamma}{4} \right) = \frac{\delta}{2}.$$
Similarly, if $\xi_{kj}^n < \xi_{ij}^n$, we get $\xi_{ij}^n \leq \frac{\delta}{2}$. Combining the two cases, we have that $w_{ij}^n \leq \frac{\delta}{2}$, which gives the desired contradiction that proves that $T_n = T$ if $(6.8)$ holds in some realization of the data.

Now note that by assumption, we have that for all $i, j \in V$,

$$|E(\xi_{ij}^n) - \xi_{ij}| \leq \frac{\delta^2}{8} \leq \frac{\delta^2(2 - \delta)}{8} = \frac{\gamma}{8}.$$  

Thus, for $(6.8)$ to hold, it suffices that we have

$$|\xi_{ij}^n - E(\xi_{ij}^n)| \leq \frac{\gamma}{8} \text{ for all } i, j.$$ 

To prove the required bound, it is therefore sufficient to show that for any distinct $i, j \in V$,

$$P\left(|\xi_{ij}^n - E(\xi_{ij}^n)| > \frac{\gamma}{8}\right) \leq C_1(\delta)e^{-C_2(\delta)n},$$

where $C_1(\delta)$ and $C_2(\delta)$ are positive constants that depend only on $\delta$. By Proposition [6.1], this holds if we replace $\gamma/8$ on the left side by any $t \in [0, C_3(\delta)]$, where $C_3(\delta)$ is another positive constant that depends only on $\delta$, and insert $t^2$ inside the exponent on the right. Taking $t = \min\{\gamma/8, C_3(\delta)\}$, and observing the left side can only increase if we replace $\gamma/8$ by $t$, we get the desired result.

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