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BOUNDS AND HOMOTOPY IN PREDICTION**

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# Maximal Association, Fréchet Bounds and Homotopy in Prediction

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## Abstract:

Suppose we want to know about a random quantity  $X_1$  which is hard to observe. On the other hand, we have  $(X_2, X_3)$  which is of easy observation and is believed to bring information about  $X_1$ . We want to establish how much we can expect of  $(X_2, X_3)$  being able to predict  $X_1$ . We study the problem under the maximal association which is related to the Fréchet Bounds. We also study a homotopy related to the problem.

**Keywords:** Fréchet Bounds; Kendall's  $\tau$ ; Negative and Positive, TP2 and RR2 Associations; Copula; Homotopy.

## 1. Introduction

In this work we deal with the following type of problem: suppose we want to know about a random quantity  $X_1$  which is observable after some relevant degree of difficulty. On the other hand, we have  $(X_2, X_3)$  which is of easy observation (easier than  $X_1$ ) and is believed to bring information about  $X_1$ . The information is in the sense that it is expected to exist a strong association between  $X_1$  and  $(X_2, X_3)$ . Under the formalization of the association we want to establish how much we can expect of  $(X_2, X_3)$  being able to predict  $X_1$ . The first motivation to this problem was the situation of an expert having to infer the health condition of a patient from a bunch of clinical results. Indeed, the desirable version of this problem would be to consider both  $X_1$  and  $(X_2, X_3)$  being general multivariate vectors. However, for the type of

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results we have and for the time being, we can only deal with this simple situation.

In our problem the more convenient definitions of dependency are:

**Definition 1.1.** We say that a random vector  $\underline{X} = (X_1, X_2, \dots, X_n)$  is

- i. *Negative Associated (NA)* [Proschan and Joag-Dev(1983)] if for every pair of disjoint subsets  $A_1, A_2$  of  $\{1, 2, \dots, n\}$ , where  $A_1 = \{i_1, \dots, i_k\}$ ,  $A_2 = \{i_{k+1}, \dots, i_n\}$ ,  $i_s < i_t$  for  $s < t$  and for every pair of increasing functions  $f$  and  $g$  from  $\mathbb{R}^k$  and  $\mathbb{R}^{n-k}$ , respectively, to  $\mathbb{R}$ , we have

$$\text{Cov}(f(X_i, i \in A_1), g(X_j, j \in A_2)) \leq 0.$$

- ii. *Pairwise Negative Associated (PNA)* if every pair of its distinct coordinates is negative associated.

**Definition 1.2.** We say that a random vector  $\underline{X} = (X_1, X_2, \dots, X_n)$  is

- i. *Positive Associated (PA)* [Joag-Dev(1983)] if for every pair of increasing (coordinatewise) functions  $f$  and  $g$  on  $\mathbb{R}^n$  we have

$$\text{Cov}(f(\underline{X}), g(\underline{X})) \geq 0.$$

- ii. *Pairwise Positive Associated (PPA)* if for every pair of its distinct coordinates is positive associated.

As can be noticed, the two above definitions are not converse to each other. The NA definition is closed under increasing functions, each of such functions being defined on disjoint subsets of variables composing a NA vector. In fact, among all types of negative dependencies, the NA is the only one to satisfy such property (see Joag-Dev and Proschan(1983)). Meanwhile, the PA concept appears as a generalization to the concept of positively correlated random variables.

Much has already been done towards exploring several different types of dependencies, their applications and interpretations in different areas like Survival Analysis, Reliability and Multivariate Analysis. Among several related works we mention Joag-Dev and Proschan(1983), Block, Savits and Shaked(1982), Ebrahimi and Ghosh(1981), Boland, Hollander, Joag-Dev and Kochar(1996) and Joe(1997).

**Definition 1.3.** [Karlin and Rinott(1980)a, b] Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  be a non-negative function.

i. We say  $f$  is a multivariate totally positive function of order 2 (MTP2) if

$$f(x \vee y)f(x \wedge y) \geq f(x)f(y)$$

for any  $x$  and  $y$  in  $\mathbb{R}^n$  and

$$x \vee (\wedge) y = (\max(\min)\{x_1, y_1\}, \max(\min)\{x_2, y_2\}, \dots, \max(\min)\{x_n, y_n\}).$$

When  $n = 2$  we say  $f$  is totally positive function of order 2 (TP2).

ii. We say that  $f$  is multivariate reverse rule of order 2 (MRR2) if

$$f(x \vee y)f(x \wedge y) \leq f(x)f(y)$$

for any  $x$  and  $y$  in  $\mathbb{R}^n$ . When  $n = 2$  we say that  $f$  is reverse rule of order 2 (RR2).

**Definition 1.4.** Let  $\underline{X} = (X_1, X_2, \dots, X_n)$  be a random vector with density function  $f_{\underline{X}}$ . We say that  $\underline{X}$  is MTP2(MRR2) if  $f_{\underline{X}}$  is MTP2(MRR2).

Karlin and Rinott(1980a, b) give a detailed study of TP2 and RR2 concepts for bivariate densities and then generalize it for n-variate densities. Among other things, it is shown there that TP2 implies PA, as well as, that RR2 implies NA. This last result was also proven by Joag-Dev and Proschan(1983). Therefore, we can restrict the PA(NA) condition to the class of TP2(RR2) densities making sense of the following definitions:

**Definition 1.5.**

- a. If  $X$  and  $Y$  are two random variables then we say they are PA(TP2) if their joint density function is TP2.
- b. If  $X$  and  $Y$  are two random variables then we say they are NA(RR2) if their joint density function is RR2.

Although the PA and NA definitions are weaker than the PA(TP2) and NA(RR2) ones we are going to stick to the last two ones because if we are to deal with the problem of predicting  $X_1$  from  $(X_2, X_3)$  then we need to quantify the dependencies between  $X_1$  and  $X_i$  for  $i = 2, 3$  and using the last definitions we can use an already existing measure of such dependencies known as Kendall's  $\tau$ .

**Definition 1.6.** Let  $(X'_1, X'_2)$  and  $(X''_1, X''_2)$  be two pairs of random variables, both having distribution  $P$ . The Kendall's  $\tau$  measure is defined as

$$\tau_{X_1, X_2} = P\{(X'_1 - X''_1)(X'_2 - X''_2) \geq 0\} - P\{(X'_1 - X''_1)(X'_2 - X''_2) < 0\}.$$

The description of Kendall's  $\tau$  as a measure of association in this case is given by the following result:

**Theorem 1.7.** [Nelsen(1992)] Let  $X_1$  and  $X_2$  be two random variables with absolute continuous joint distribution function  $F_{X_1, X_2}$  associated to the joint density function  $f_{X_1, X_2}$ . Let  $T_{X_1, X_2}$  be the "local" measure mean of the TP2(RR2) condition defined as

$$T_{X_1, X_2} := \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{x'_2} \int_{-\infty}^{x'_1} \{f_{X_1, X_2}(x'_1, x'_2)f_{X_1, X_2}(x_1, x_2) - f_{X_1, X_2}(x'_1, x_2)f_{X_1, X_2}(x_1, x'_2)\} dx_1 dx_2 dx'_1 dx'_2.$$

(Implicitly we are assuming  $-\infty < x_i < x'_i < +\infty$ ,  $i = 1, 2$ .) Then

$$T_{X_1, X_2} = \frac{\tau_{X_1, X_2}}{2}.$$

In words, if  $f_{X_1, X_2}$  is TP2(RR2) then  $\tau_{X_1, X_2}$  is a measure of association TP2(RR2) in the sense that  $\tau_{X_1, X_2}$  is twice the mean of "local" measure of the TP2(RR2) condition.

In Kruskal(1958) we have the notion that  $\tau_{X_1, X_2}$  measures the agreement/disagreement between  $X_1$  and  $X_2$ . One important feature of such measure is its invariance with respect to concordant monotone transformations, i.e., if  $f$  and  $g$  are two transformations, either both monotonically increasing or both decreasing then  $\tau_{h(X_1), g(X_2)} = \tau_{X_1, X_2}$ . If  $X_1$  and  $X_2$  are independent then  $\tau_{X_1, X_2} = 0$  but the converse is not true in general.

In this work we study the effectiveness of Kendall's  $\tau$  as a measure of the information  $Y$  brings to  $X$  meaning with this the notion that the greater the absolute value of the  $\tau$  measure the greater the association between the two random variables. In the context of our problem that is to say: if the pair  $(X_1, X_2)$  exhibits absolute  $\tau$  value greater than the pair  $(X_1, X_3)$  then  $X_2$  brings more information about  $X_1$  than  $X_3$  does. We give the characterization of complete association when Kendall's  $\tau$  assumes the extreme values, either  $+1$  or  $-1$ . This is done in two steps. First, we deal with the

case  $(X_1, X_2)$  having uniform on  $[0, 1]$  distributed marginals. Then we use results in de Finetti(1953) and in Esteves, Wechsler, Leite and Gonzalez-Lopez(1999) to extend such result to the case of continuous distribution functions with general marginals. For intermediate values of  $\tau$  we give some partial results.

Following the type of results in Esteves, Wechsler, Leite and Gonzalez-Lopez(1999) we exploit the idea that if  $(X_1, X_2, \dots, X_n)$  is a random vector with continuous distribution function  $F$  then  $V = F(\infty, X_2, \dots, X_n)$ , uniformly distributed, constitutes a valuable summary of  $(X_2, X_3, \dots, X_n)$  in order to infer about  $X_1$ . We establish the conditions under which such happens.

The other result we will see is related to the Fréchet Bounds which goes back to Fréchet(1951), namely, if  $F_{U_1, U_2}$  is the joint distribution function of  $(U_1, U_2)$  with marginals  $F_{U_1}$  and  $F_{U_2}$  then

$$\max\{F_{U_1}(u_1) + F_{U_2}(u_2) - 1, 0\} \leq F_{U_1, U_2}(u_1, u_2) \leq \min\{F_{U_1}(u_1), F_{U_2}(u_2)\}, \\ \forall (u_1, u_2) \in \mathbb{R}^2.$$

**Definition 1.8** *A subset  $S$  of  $\mathbb{R}^2$  is non-decreasing if and only if for all  $(x, y), (u, v)$  in  $S$ ,*

$$x < u \Rightarrow y \leq v.$$

It was shown by Mikusinski, Sherwood and Taylor(1991-92) that  $F_{U_1, U_2}$  attains the maximal bound if and only if there is a non-decreasing subset  $D \subset \mathbb{R}^2$  so that  $(U_1, U_2)$  is almost surely concentrated in  $D$ . This result is going to be used later.

**Definition 1.9.** *If  $F_{X_i}$ ,  $i = 1, 2, \dots, n$  are marginal distribution functions then we define the Fréchet class related to  $\{F_{X_i}\}_{i=1}^n$  as being the set of joint distribution functions whose marginals are  $F_{X_i}$ ,  $i = 1, 2, \dots, n$ .*

Joe(1997) makes a careful study about the Fréchet Classes. He goes further than associating the joint distribution and its marginals (and possible inferences from there). He also establishes connection between one Fréchet Class and a set of given multivariate marginals. For instance, he deals with problems like: if we have a set of bivariate marginals  $F_{X_i, X_j}$ ,  $i \neq j$ ,  $i, j \in \{1, 2, \dots, n\}$  then how to characterize one joint distribution function having such given functions as some of its marginals? He also deals with conditional joint distribution functions, which makes the construction of the associated

Fréchet Class more realistic and indeed more mathematically involved. In some cases the given marginals satisfy relationships established through their Kendall's  $\tau$  measures. Following those lines, if we assume that the joint distribution function  $F$  is the best function to explain the dependencies among the variables  $X_1, X_2, \dots, X_n$  then one can ask:

- How the relationships among the variables are going to be if their joint distribution function is given by one of the two Fréchet Bounds?
- How can we relate  $F$  to either the upper or the lower Fréchet Bounds of the class to which  $F$  belongs?

The answers to the first question in the bivariate case are given in Section 2. Trying to answer the second question we check what if  $F$  is a perturbation of either the upper or the lower Fréchet Bound? We consider the homotopy  $H(t) = (1 - t)F + t \min\{F_{X_1}, F_{X_2}\}$  with  $t$  close to one for the upper Fréchet Bound. (For details on homotopy from the viewpoint we use see Joe(1997) and references therein.) Using such  $H$ , in Section 3 we show that if  $F_{X_1, X_2}$  is a continuous distribution function with uniformly distributed marginals then  $F_{X_1, X_2}$  can be continuously transformed in to the maximal Fréchet bound associated to its Fréchet Class. Given a Fréchet class related to  $\{F_{X_1}, F_{X_2}\}$  then the Fréchet bounds  $\max\{F_{X_1}(x_1) + F_{X_2}(x_2) - 1, 0\}$  and  $\min\{F_{X_1}(x_1), F_{X_2}(x_2)\}$  are respectively the distributions with maximum negative and positive association in the class. We would then conjecture that for general  $F_{X_1, X_2}$  it is possible to go continuously from it to one of the Fréchet Bounds. Which bound would depend on the association of the original vector  $(X_1, X_2)$  being positive or negative.

We will need the concept of copula which we define now.

**Definition 1.10.** [Sklar(1959), Joe(1997)] Let  $\underline{X} = (X_1, X_2, \dots, X_n)$  be a random vector with distribution function  $F_{\underline{X}}$  whose marginals are given by  $F_{X_1}, \dots, F_{X_n}$ . We define the copula associated to  $F_{\underline{X}}$  as a distribution function  $C_{\underline{X}} : \mathbb{I}^n \rightarrow \mathbb{I}$ , with uniform  $[0, 1]$  marginals and satisfying,

$$F_{\underline{X}}(\underline{x}) = C_{\underline{X}}(F_{X_1}(x_1), \dots, F_{X_n}(x_n)), \forall \underline{x} = (x_1, \dots, x_n) \in \mathbb{R}^n.$$

The rest of this paper is organized as follows. In Section 2 we give the definitions and the results. In Section 3 we discuss the Fréchet Classes, the Fréchet Bounds and homotopy. In Section 4 we prove the results in Section 2.

## 2. Notations and results

### 2.1. Kendall's $\tau$ and maximum positive association

We describe next the results we have connecting the maximum positive association and Kendall's  $\tau$ .

**Proposition 2.1.1.** *Suppose the random variables  $X_1, X_2$  have the joint distribution  $F_{X_1, X_2}$  whose marginals are  $U[0, 1]$ . Then the following conditions are equivalent:*

- i.  $\tau_{X_1, X_2} = 1$
- ii.  $P\{X_1 = X_2\} = 1$
- iii.  $F_{X_1, X_2}(x_1, x_2) = \min\{x_1, x_2\}$  for  $x_1, x_2 \in \mathbb{I} = [0, 1]$
- iv.  $X_2 = f(X_1)$  a.e.  $[P]$  for some non-decreasing function  $f$ .

**Corollary 2.1.2.** *Let  $X_1, X_2, X_3$  be random variables and  $\varphi : \mathbb{R}^2 \rightarrow \mathbb{R}$  be a mapping so that  $X_1$  and  $\varphi(X_2, X_3)$  are both uniformly distributed on  $[0, 1]$ . Then the following conditions are equivalent:*

- i.  $\tau_{X_1, \varphi(X_2, X_3)} = 1$
- ii.  $P\{X_1 = \varphi(X_2, X_3)\} = 1$
- iii.  $F_{X_1, \varphi(X_2, X_3)}(x_1, x_2) = \min\{F_{X_1}(x_1), F_{\varphi(X_2, X_3)}(x_2)\}$  for  $x_1, x_2 \in \mathbb{I} = [0, 1]$
- iv.  $\varphi(X_2, X_3) = f(X_1)$  a.e.  $[P]$  for some non-decreasing function  $f$ .

The previous corollary gains relevance if we recall a de Finetti(1953) result, namely, if  $X_2$  and  $X_3$  have a joint continuous distribution then there exists a function  $\varphi : \mathbb{R}^2 \rightarrow \mathbb{R}$  so that  $\varphi(X_2, X_3)$  has uniform distribution. Proposition 2.1.1 can then be rewritten by using a copula associated to the joint distribution  $F_{X_2, X_3}$ . In fact, when we have maximum positive association, as in this case, the copula is well defined and it is a Fréchet bound.

**Corollary 2.1.3.** *Suppose  $X_1, X_2$  have joint distribution  $F_{X_1, X_2}$  whose marginals  $F_{X_1}, F_{X_2}$  are continuous. Then the following conditions are equivalent:*



- i.  $\tau_{X_1, X_2} = 1$
- ii.  $F_{X_1, X_2}(x_1, x_2) = \min\{F_{X_1}(x_1), F_{X_2}(x_2)\}$  for  $x_1, x_2 \in \mathbb{I} = [0, 1]$
- iii.  $F_{X_2}(X_2) = f \circ F_{X_1}(X_1)$  a.e.  $[F_{X_1, X_2}]$  for some non-decreasing function  $f$ .

We use next a result in Esteves, Wechsler, Leite and Gonzalez-Lopez (1999) credited to de Finetti(1953), namely, let  $X_1$  and  $U$  be random variables with continuous distribution functions  $F_{X_1}$  and  $F_U$  respectively. Then, there exists a function  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  such that  $\phi(X_1)$  and  $\phi(U)$  are both uniformly distributed on  $[0, 1]$ . This and Corollary 2.1.3 give us the following

**Proposition 2.1.4.** *Let  $X_1$  be a random variable with continuous distribution function  $F_{X_1}$  and  $X_2, X_3$  be two random variables with joint continuous distribution  $F_{X_2, X_3}$ . Then,*

- a) *there exists  $\varphi_1 : \mathbb{R} \rightarrow \mathbb{R}$  and  $\varphi_{2,3} : \mathbb{R}^2 \rightarrow \mathbb{R}$  so that  $\varphi_1(X_1)$  and  $\varphi_{2,3}(X_2, X_3)$  are both  $U[0, 1]$  distributed;*
- b) *if we define  $U = \varphi_1(X_1)$  and  $V = \varphi_{2,3}(X_2, X_3)$  then the following are equivalent:*
  - b1)  $F_{U,V}(u, v) = \min\{F_U(u), F_V(v)\}$
  - b2)  $\tau_{U,V} = 1$ .

There are some topological difficulties in order to get the function  $\varphi_1$  as pointed out by Esteves, Wechsler, Leite and Gonzalez-Lopez(1999). For such reason we suggest the use of  $\varphi_1 = F_{X_1}$  reminding the invariance property of Kendall's  $\tau$  with respect to monotone non-decreasing transformations.

The statistical relevance of the above results can be seen in the following way: if  $X_1$  is to be predicted from  $(X_2, X_3)$  then it is possible to work in the domain of joint distributions with uniform marginals when  $\varphi_1, \varphi_1^{-1}$  and  $\varphi_{2,3}$  are obtainable. This change of domain may be important, for instance, when dealing with data in the computer.

## 2.2. Maximum negative association

In the case of maximum negative association the results become:

**Proposition 2.2.1.** *Suppose  $X_1$  and  $X_2$  are r. v. with joint distribution  $F_{X_1, X_2}$  with uniform marginals. Then the following conditions are equivalent*

- i.  $\tau_{X_1, X_2} = -1$
- ii.  $P\{X_2 = 1 - X_1\} = 1$
- iii.  $F_{X_1, X_2}(x_1, x_2) = \max\{0, x_1 + x_2 - 1\}$ ,  $x_1, x_2 \in \mathbb{I}$
- iv.  $X_2 = f(X_1)$  a.e.  $[P]$  for some non-increasing function  $f$ .

**Corollary 2.2.2.** *If  $X_1, X_2, X_3$  are r. v.'s,  $\varphi : \mathbb{R}^2 \rightarrow \mathbb{R}$  a mapping,  $X_1$  and  $\varphi(X_2, X_3)$  are uniformly distributed on  $[0, 1]$  then the following conditions are equivalent:*

- i.  $\tau_{X_1, \varphi(X_2, X_3)} = -1$
- ii.  $P\{\varphi(X_2, X_3) = 1 - X_1\} = 1$
- iii.  $F_{X_1, \varphi(X_2, X_3)}(x_1, x_2) = \max\{0, F_{X_1}(x_1) + F_{\varphi(X_2, X_3)}(x_2) - 1\}$ ,  $x_1, x_2 \in \mathbb{I}$
- iv.  $\varphi(X_2, X_3) = f(X_1)$  a.e.  $[P]$  for some non-increasing function  $f$ .

By invariance of Kendall's  $\tau$  to monotone transformations we can consider taking  $\varphi_1(X_1)$  instead of  $X_1$  so that  $\varphi_1(X_1)$  is uniformly distributed on  $(0, 1)$ . Again, in order to avoid topological annoyances, we suggest the use of  $\varphi_1(X_1) = F_{X_1}(X_1)$ .

### 2.3. Kendall's $\tau$ and association comparison

**Definition 2.3.1.** *Let  $(X_1, X_2)$  and  $(X_1, X_3)$  be two pairs of r. v.'s having probability density functions  $f_{X_1, X_2}$  and  $f_{X_1, X_3}$ , both TP2 type. We say  $(X_1, X_2)$  is locally positive more associated than  $(X_1, X_3)$  in a TP2 sense if*

$$\begin{aligned} f_{X_1, X_2}(x', y') f_{X_1, X_2}(x, y) &- f_{X_1, X_2}(x', y) f_{X_1, X_2}(x, y') \geq \\ f_{X_1, X_3}(x', y') f_{X_1, X_3}(x, y) &- f_{X_1, X_3}(x', y) f_{X_1, X_3}(x, y') \end{aligned}$$

for any  $(x', x, y', y)$  satisfying  $x' \geq x, y' \geq y$ .

**Definition 2.3.2.** *Let  $(X_1, X_2)$  and  $(X_1, X_3)$  be two pairs of r. v.'s having probability density functions  $f_{X_1, X_2}$  and  $f_{X_1, X_3}$ , both TP2 type. We say  $(X_1, X_2)$  is positively more associated than  $(X_1, X_3)$  in a TP2 sense if*

$$\tau_{X_1, X_2} \geq \tau_{X_1, X_3}.$$

As we learned from Nelsen(1992), when probability density functions exist,  $\tau$  is an TP2 association measure, and in this case, locally positive more association implies global positive association.

Let  $(X_1, X_2, \dots, X_n)$  be a random vector with probability density function  $f_{X_1, X_2, \dots, X_n}$  and let  $U$  be a function of  $X_2, X_3, \dots, X_n$ . We want to know under what conditions we have

$$\tau_{X_1, U} = \tau_{X_1, \varphi(X_2, \dots, X_n)} \geq \max_{2 \leq k \leq n} \{\tau_{X_1, X_k}\}.$$

We should remark that the use of Kendall's  $\tau$  to choose the function of  $(X_2, \dots, X_n)$  to be used to make inference about  $X_1$  forces the restriction to the class of functions  $\varphi: \mathbb{R}^{n-1} \rightarrow \mathbb{R}$  since the  $\tau$  measure is only well defined for univariate random variables. If we want to measure the agreement of three or more random quantities then we can, for instance, specify one particular direction in the space of  $(X_2, \dots, X_n)$  where maximization of  $\tau$  will be taken into account.

On the other hand, we can have the situation where none of the quantities  $X_i, i = 2, \dots, n$ , marginally provide a satisfactory inference about  $X_1$ . One possible strategy in this case is trying to gather all the contributions, putting together all the variables, jointly with their relationships. Specifically, we need a function assuming values in  $\mathbb{R}$  which is sensitive to all variations of the behavior of the vector  $(X_1, X_2, \dots, X_n)$ . One such candidate is the cumulative joint distribution function  $F_{(X_2, \dots, X_n)}$ . Naturally, then, we need to know under what conditions the choice of  $U_2 = F_{(X_2, \dots, X_n)}(X_2, \dots, X_n)$  is sound when the  $\tau$  measure is used as a criteria in the selection. In words, if  $X_1$  is to be predicted from  $X_2, X_3, \dots, X_n$  then under what conditions a function of them jointly is better than using each of them separately? First, let us see a preliminary result.

**Lemma 2.3.3.** *Let  $\underline{X} = (X_1, X_2, \dots, X_n)$  be a random vector with continuous distribution function  $F_{\underline{X}}$ . Suppose that there exists an ordered sequence of sub-indices  $\{i_1, i_2, \dots, i_{n-1}\} \subset \{1, 2, \dots, n\}$  so that the conditional probability  $P\{\omega : F_{\underline{X}}(\underline{X}(\omega)) = u | X_{i_1} = x_{i_1}^0, \dots, X_{i_{n-1}} = x_{i_{n-1}}^0\}$  is non-trivially well defined (in the sense of not being zero) for every  $(x_{i_1}^0, \dots, x_{i_{n-1}}^0)$  on the image of  $(X_{i_1}, \dots, X_{i_{n-1}})$  and every  $u \in (0, 1)$ . Then the random variable  $U = F_{\underline{X}}(X_1, \dots, X_n)$  has a continuous distribution function.*

Using the last result we can get the following

**Proposition 2.3.4.** *Let  $\underline{X} = (X_1, \dots, X_n)$  be a random vector so that  $F_{X_1}$  and  $F_{X_2, \dots, X_n}$  are continuous and  $F_{X_2, \dots, X_n}$  has an ordered sequence of sub-indices as in the previous lemma. Suppose that if  $(X_2, \dots, X_n)$  and  $(X'_2, \dots, X'_n)$  are two independent vectors with the same distribution  $F_{X_2, \dots, X_n}$  then they satisfy*

- i.  $X_i \geq X'_i$  and  $X_j \geq X'_j \Rightarrow X_s \geq X'_s, \quad \forall i, j, s \in \{2, 3, \dots, n\}, \quad i \neq j, i \neq s, j \neq s.$
- ii.  $\{(X_i - X'_i)(X_j - X'_j) < 0\} \Rightarrow \{(X_j - X'_j)(U_2 - U'_2) < 0\} \quad \forall i, \forall j \in \{2, \dots, n\}, i \neq j.$

In words, in (i) we have agreement of tendencies and in (ii), if two coordinates disagree then  $U_2 - U'_2 = F_{X_2, \dots, X_n}(X_2, \dots, X_n) - F_{X_2, \dots, X_n}(X'_2, \dots, X'_n)$  also disagrees with one of the coordinates. Under such hypotheses we have that

$$\tau_{X_1, U_2} \geq \max_{2 \leq i \leq n} \{\tau_{X_1, X_i}\}.$$

From this proposition it immediately follows

**Corollary 2.3.5.** *Let  $\underline{X} = (X_1, \dots, X_n)$  with associated  $F_{X_1}$  and  $F_{X_2, \dots, X_n}$  being continuous and  $F_{X_2, \dots, X_n}(X_2, \dots, X_n)$  being a continuous distribution function. If  $X_1$  and  $X_i$  are Positive Associated (TP2) for  $i = 2, \dots, n$  then*

$$\tau_{X_1, U_2} \geq \max_{2 \leq i \leq n} \{\tau_{X_1, X_i}\}.$$

Recall that under the hypotheses we are assuming Kendall's  $\tau$  is a measure of association.

Given the above result, in order to predict  $X_1$ , instead of using only one of  $X_2, \dots, X_n$  it is better to use

$$F_{X_1}^{-1}(U_2) = F_{X_1}^{-1}(F_{X_2, \dots, X_n}(X_2, \dots, X_n))$$

at least under the criteria of maximizing association.

**Open problem:** Is there a scalar function  $\varphi_0(X_2, \dots, X_n)$  which makes true

$$\tau_{X_1, \varphi_0} \geq \tau_{X_1, \varphi(X_{i_1}, \dots, X_{i_h})}$$

for any  $(X_{i_1}, \dots, X_{i_h}) \subset (X_1, \dots, X_n)$  and any  $\varphi : \mathbb{R}^k \rightarrow \mathbb{R}$ , for some  $k \leq n$ , when  $(X_1, X_2, \dots, X_n)$  belongs to some convenient class of multivariate distributions?

### 3. Homotopy as a connection between joint distribution functions

#### 3.1. Homotopic mappings

**Definition 3.1.1.** Let  $E_1$  and  $E_2$  be two topological spaces and  $I = [0, 1] \subset \mathbb{R}$ . Let  $f, g : E_1 \rightarrow E_2$  be two continuous mappings. We say  $f$  and  $g$  are homotopic when there exists a continuous application  $H : E_1 \times I \rightarrow E_2$  so that for each  $x_1 \in E_1$ ,  $H(x_1, 0) = f(x_1)$  and  $H(x_1, 1) = g(x_1)$ .  $H$  in this case is called to be an homotopy between  $f$  and  $g$ .

**Definition 3.1.2.** Let  $C(E_1, E_2)$  denote the set of continuous applications from  $E_1$  to  $E_2$ . The topology in  $C(E_1, E_2)$  generated by the sets of the form  $A(K, V) := \{f \in C(E_1, E_2) : f(K) \subseteq V\}$   $K \subset E_1$ ,  $K$  compact and  $V \subset E_2$ ,  $V$  open, is called the open-compact topology and the corresponding topological space is denoted by  $C_{OC}(E_1, E_2)$ .

It is well known that if  $E_1$  is a locally compact Hausdorff space then  $f$  and  $g$  are homotopic if and only if they belong to the same connected component in  $C_{OC}(E_1, E_2)$ . Such components are called the homotopy class of mappings from  $E_1$  to  $E_2$ .

#### 3.2. The connection between $F_{U_1, U_2}$ and the maximal Fréchet bound

From now on we consider  $\mathbb{R}^2$  with the usual topology.  $F_{U_1, U_2}$  is an absolute continuous joint distribution function whose marginals are uniformly distributed on  $(0, 1)$ . Indeed,  $F_{U_1, U_2}$  is a copula. The maximal copula is given by  $\min\{u_1, u_2\}$ . It is possible to encompass both distributions by a homotopy

$$H : \mathbb{R}^2 \times [0, 1] \rightarrow [0, 1]$$

so that

$$\begin{aligned} H((u_1, u_2), 0) &= F_{U_1, U_2}(u_1, u_2) \\ H((u_1, u_2), 1) &= \min\{u_1, u_2\}. \end{aligned} \tag{1}$$

The required boundary conditions are:

$$\begin{aligned}
F_{U_1, U_2}(u_1, 0) &= \min\{u_1, 0\} = 0, & \forall u_1 \in [0, 1] \\
F_{U_1, U_2}(u_1, 1) &= \min\{u_1, 1\} = u_1, & \forall u_1 \in [0, 1] \\
F_{U_1, U_2}(0, u_2) &= \min\{0, u_2\} = 0, & \forall u_2 \in [0, 1] \\
F_{U_1, U_2}(1, u_2) &= \min\{1, u_2\} = u_2, & \forall u_2 \in [0, 1].
\end{aligned} \tag{2}$$

The application which solves the problem is given by

$$H((u_1, u_2), t) := (1 - t)F_{U_1, U_2}(u_1, u_2) + t \min\{u_1, u_2\},$$

for  $t \in [0, 1]$  and  $u_i \in [0, 1]$ ,  $i = 1, 2$ .

It is easy to check that such  $H$  satisfies both (1) and (2) conditions. Moreover,  $H$  is continuous on  $(u_1, u_2)$  since both  $F_{U_1, U_2}(u_1, u_2)$  and  $\min\{u_1, u_2\}$  are continuous. Also,  $H$  is continuous in  $t$  since it is a linear transformation.

We have then learned that we can deform  $F_{U_1, U_2}$  in a continuous way to  $\min\{u_1, u_2\}$  by using  $H$ : for each  $(u_1, u_2) \in [0, 1]^2$  the point  $F_{U_1, U_2}(u_1, u_2)$  is slid along the line segment  $[F_{U_1, U_2}(u_1, u_2), \min\{u_1, u_2\}]$  when  $t$  grows in  $[0, 1]$ . Such homotopy is called linear and the paths  $F_{U_1, U_2}(u_1, u_2)$  and  $\min\{u_1, u_2\}$  are said to be linearly homotopic.

**Proposition 3.2.1.** *For each  $t \in [0, 1]$  fixed,  $H((\cdot, \cdot), t)$  is a continuous distribution function.*

**Proof:** It is enough to notice that  $F_{U_1, U_2}(u_1, u_2) \leq \min\{u_1, u_2\}$ ,  $\forall u_i \in [0, 1]$ ,  $i = 1, 2$  to conclude that attributes non-null probability to each set of type  $(a, b] \times (c, d] \subseteq [0, 1]^2$ . ■

**Example:** The homotopy

$$C(u, v, t) = t \min\{u, v\} + (1 - t)uv, \quad \forall t \in [0, 1], \quad u, v \in [0, 1]$$

has already appeared in Joe((1997), p. 148). In this case, the homotopy transforms continuously the path  $uv$  ( the independent copula) in to the path  $\min\{u, v\}$  ( the maximum association copula). ■

## 4. Proofs of the results

### 4.1. Proof of Proposition 2.1.1

(i)  $\Rightarrow$  (ii):

As  $(X_1, X_2)$  has uniform $[0, 1]$  marginals we can write

$$P\{X_1 > x_1, X_2 > x_2\} = F_{X_1, X_2}(x_1, x_2) - x_1 - x_2 + 1,$$

for  $0 \leq x_1, x_2 \leq 1$ .

If  $(X_1, X_2)$  and  $(X'_1, X'_2)$  are two independent realizations following  $F_{X_1, X_2}$  then

$$\begin{aligned} \tau_{X_1, X_2} &= P\{(X'_1 - X_1)(X'_2 - X_2) > 0\} = \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [P\{X'_1 > x_1, X'_2 > x_2\} + \\ &P\{X'_1 < x_1, X'_2 < x_2\} + P\{X'_1 = x_1\} + \\ &P\{X'_2 = x_2\} - P\{X'_1 = x_1, X'_2 = x_2\}] dF_{X_1, X_2}(x_1, x_2) = \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [2F_{X_1, X_2}(x_1, x_2) - x_1 - x_2 + 1] dF_{X_1, X_2}(x_1, x_2) \end{aligned}$$

where the last equality is justified by  $(X_1, X_2)$  having uniform marginals.

But then, by the hypothesis, this means  $2F_{X_1, X_2}(x_1, x_2) - x_1 - x_2 + 1 = 1$  which implies

$$F_{X_1, X_2}(x_1, x_2) = \frac{x_1 + x_2}{2}$$

for  $(x_1, x_2) \in (0, 1)^2$ .

On the other hand,  $F_{X_1, X_2}$ , having uniform distribution, has the Fréchet bound from above,

$$F_{X_1, X_2}(x_1, x_2) \leq \min\{x_1, x_2\}$$

for  $(x_1, x_2) \in (0, 1)^2$ .

Putting the two results above together, it implies that  $X_1 = X_2$  a.s. [P].

(ii)  $\Rightarrow$  (iii):

$$\begin{aligned} F_{X_1, X_2}(x_1, x_2) &= P\{X_1 \leq x_1, X_2 \leq x_2\} = \\ &= P\{X_1 \leq x_1, X_2 \leq x_2, X_1 = X_2\} = \\ &= P\{X_1 \leq \min\{x_1, x_2\}\} = \min\{x_1, x_2\} \end{aligned}$$

where the second equality follows from hypothesis and the last one from the uniformity of the marginals.

(iii)  $\Rightarrow$  (iv):

It is proven, for example, in Mikusinski, Sherwood and Taylor(1991-1992). In fact, it is shown there that (iii) and (iv) are equivalent, using the concept of non-decreasing subset  $S$  of  $\mathbb{R}^2$  mentioned in the introduction.

(iv)  $\Rightarrow$  (i):

Defining  $\eta_{X_1, X_2} = P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0\}$  we have that  $\tau_{X_1, X_2} = 2\eta_{X_1, X_2} - 1$  where  $(X_1, X_2)$  and  $(X'_1, X'_2)$  are two independent realizations of distribution  $F_{X_1, X_2}$ . From (iv) we get that  $P\{X_2 = f(X_1), X'_2 = f(X'_1)\} = 1$  so that

$$\begin{aligned}\eta_{X_1, X_2} &= P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0, X_2 = f(X_1), X'_2 = f(X'_1)\} = \\ &P\{(X_1 - X'_1)(f(X_1) - f(X'_1)) \geq 0, X_2 = f(X_1), X'_2 = f(X'_1)\} = 1\end{aligned}$$

since  $f$  is monotone non-decreasing. ■

#### 4.2. Proof of Corollary 2.1.3

(i)  $\Rightarrow$  (ii):

By invariance property of  $\tau$  for non-decreasing functions we get that

$$1 = \tau_{X_1, X_2} = \tau_{U_1, U_2}$$

where  $U_i = F_{X_i}(X_i)$ ,  $i = 1, 2$ .

This and the previous proposition imply that

$$P\{U_1 = U_2\} = 1 \tag{3}$$

For  $x_i \in \text{Image}(X_i)$ ,  $i = 1, 2$  and  $C_{X_1, X_2}$  the copula associated to  $F_{X_1, X_2}$  it follows that

$$\begin{aligned}F_{X_1, X_2}(x_1, x_2) &= C_{X_1, X_2}(F_{X_1}(x_1), F_{X_2}(x_2)) = \\ &C_{X_1, X_2}(u_1, u_2) = F_{U_1, U_2}(u_1, u_2)\end{aligned} \tag{4}$$

with  $u_i = F_{X_i}(x_i)$ ,  $i = 1, 2$  and the last equality is a consequence of copula definition.

Then, recalling (3), it follows that

$$F_{U_1, U_2}(u_1, u_2) = \min\{u_1, u_2\} = \min\{F_{X_1}(x_1), F_{X_2}(x_2)\}.$$

(ii)  $\Rightarrow$  (iii):



Using the last equation in (4) we have that

$$F_{U_1, U_2}(u_1, u_2) = C_{X_1, X_2}(u_1, u_2) = F_{X_1, X_2}(x_1, x_2) = \min\{u_1, u_2\}$$

where in the last equality we used the hypothesis.

This in the last proposition implies that there exists a non-decreasing  $f$  satisfying  $U_2 = f(U_1)$  a.s. [P]. Rewriting this we learn that there exists a non-decreasing  $f$  so that  $F_{X_2}(X_2) = f \circ F_{X_1}(X_1)$  a.s.[P]. ■

#### 4.3. Proof of Proposition 2.2.1

Analogous to the proof to Proposition 2.1.1, unless for two small differences elaborated next.

(ii)  $\Rightarrow$  (iii):

(ii) implies

$$\begin{aligned} P\{X_1 \leq x_1, X_2 \leq x_2\} &= P\{1 - x_2 \leq X_1 \leq x_1\} = \\ &= \begin{cases} x_1 - (1 - x_2) & \text{if } 0 \leq 1 - x_2 < x_1 \leq 1 \\ 0 & \text{otherwise} \end{cases} \\ &= \max\{0, x_1 + x_2 - 1\} \end{aligned}$$

(iv)  $\Rightarrow$  (i):

For a non-increasing function  $f$  it follows that

$$\tau_{X_1, X_2} = -P\{(X'_1 - X_1)(f(X'_1) - f(X_1)) < 0\} = -1. \quad \blacksquare$$

#### 4.4. Proof of Lemma 2.3.3

It suffices to prove the  $n = 2$  case. For  $n > 2$  the proof follows in a very similar way.

We want to show that for every  $u \in (0, 1)$ ,

$$P\{F_{X_1, X_2}(X_1, X_2) = u\} = 0.$$

For any arbitrary  $u \in (0, 1)$  we write up

$$\begin{aligned} P\{F_{X_1, X_2}(X_1, X_2) = u\} &= \int_{-\infty}^{\infty} P\{F_{X_1, X_2} = u \mid X_2 = y\} dF_{X_2}(y) \\ &= \int_{-\infty}^{\infty} \frac{P\{F_{X_1, X_2}(X_1, y) = u, X_2 = y\}}{P\{X_2 = y\}} dF_{X_2}(y) \end{aligned}$$

where the term inside the integration makes sense by hypothesis.

Let us look at  $P\{F_{X_1, X_2}(X_1, y) = u\}$  for  $y \in \text{Image}(X_2)$ . We analyse the following cases:

i. If  $u > F_{X_2}(y)$  then  $u > F_{X_1, X_2}(x, y)$  for any  $x \in \mathbb{R}$ . Therefore,

$$P\{\omega : F_{X_1, X_2}(X_1(\omega), y) = u\} = 0.$$

ii. If  $u < F_{X_2}(y)$  then let us define

$$\begin{aligned} h(x) &= F_{X_1, X_2}(x, y), \quad x \in \text{Image}(X_1) \\ h^{qi}(v) &= \inf\{t : h(t) \geq v\}, \quad v \in [u, F_{X_2}(y)]. \end{aligned}$$

Note that  $\{t : h(t) \geq v\} \neq \emptyset$  since  $h(t) \rightarrow_{t \rightarrow +\infty} F_{X_2}(y) \geq v$  for any  $v \in [u, F_{X_2}(y)]$ . Thus, there exists an  $M > 0$  so that  $\forall t > M$  we have  $h(t) \geq v$ . Moreover, the set  $\{t : h(t) \geq v\}$  is bounded from below. Since,  $\lim_{x \rightarrow -\infty} F_{X_1, X_2}(x, y) = 0$ , there exists a  $t_0$  satisfying  $h(t_0) < v$  and  $t_0$  is a bound. Hence,  $\{t : h(t) \geq v\}$  has an infimum.

By the right-continuity of  $h$  it is not hard to show that

$$h^{qi}(v) \leq t \Leftrightarrow v \leq h(t) \quad (5)$$

for any  $v \in [u, F_{X_2}(y)]$  and from this we can conclude that  $h^{qi}$  is right-continuous on his domain of definition.

Now, let us take the interval  $[u, u + \varepsilon]$  with  $u + \varepsilon \in [u, F_{X_2}(y)]$ . From (5) we get that

$$u + \varepsilon > h(x) \Leftrightarrow h^{qi}(u + \varepsilon) > x.$$

Using this and (5) again we obtain

$$\begin{aligned} P\{u \leq h(X_1) < u + \varepsilon\} &= P\{h^{qi}(u) \leq X_1 < h^{qi}(u + \varepsilon)\} \\ &= F_{X_1}(h^{qi}(u + \varepsilon)) - F_{X_1}(h^{qi}(u)) \rightarrow_{\varepsilon \searrow 0} 0. \end{aligned}$$

by the right-continuity of  $h^{qi}$  and the continuity of  $F_{X_1}$ .

iii. If  $u = F_{X_2}(y)$  then

$$\begin{aligned} P\{F_{X_1, X_2}(X_1, y) = u\} &= \\ P\{F_{X_2}(y) = u, F_{X_1, X_2}(X_1, y) = u, X_2 \leq y\} &= \\ \leq P\{X_1 \in [x_0, +\infty), X_2 \leq y\} \end{aligned}$$

where  $x_0$  is a lower bound of the set  $\{x : F_{X_1, X_2}(x, y) = u\}$  and the existence of  $x_0$  is justified by the monotonicity of  $F_{X_1, X_2}$  and the fact that  $\lim_{x \rightarrow -\infty} F_{X_1, X_2}(x, y) = 0$  any  $y$ .

But then,

$$P\{X_1 \geq x_0, X_2 \leq y\} = F_{X_2}(y) - F_{X_1, X_2}(x_0, y) = 0.$$

By gathering the three cases above we conclude that

$$P\{F_{X_1, X_2}(X_1, y) = u, X_2 = y\} = 0.$$

■

#### 4.5. Proof of the Proposition 2.3.4

We consider first the case  $n = 3$ . Let  $U = F_{X_2, X_3}(X_2, X_3)$  and let  $(X_1, U)$  and  $(X'_1, U')$  be two i.i.d.'s vectors. Define  $\eta_{X_1, U} = P\{(X_1 - X'_1)(U - U') \geq 0\}$  so that  $\tau_{X_1, U} = 2\eta_{X_1, U} - 1$ .

Similarly,  $\eta_{X_1, X_i} = P\{(X_1 - X'_1)(X_i - X'_i) \geq 0\}$  and  $\tau_{X_1, X_i} = 2\eta_{X_1, X_i} - 1$ ,  $i = 2, 3$ , with  $(X_1, X_i), (X'_1, X'_i)$ ,  $i = 2, 3$  being i.i.d.'s vectors.

Then,

$$\begin{aligned} \eta_{X_1, U} &= P\{(X_1 - X'_1)(U - U') \geq 0\} = \\ &P\{(X_1 - X'_1)(X_2 - X'_2)^2(U - U') \geq 0\} \geq (e) \\ &P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0, (X_2 - X'_2)(U - U') \geq 0\} = \\ &P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0, (X_2 - X'_2)(X_3 - X'_3)^2(U - U') \geq 0\} = (7) \\ &P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0, (X_3 - X'_3)(X_2 - X'_2) \geq 0\} + \\ &P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0, (X_2 - X'_2)(X_3 - X'_3) < 0, \\ &\quad (X_3 - X'_3)(U - U') < 0\} = (8) \\ &P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0, (X_3 - X'_3)(X_2 - X'_2) \geq 0\} + \\ &P\{(X_1 - X'_1)(X_2 - X'_2) \geq 0, (X_3 - X'_3)(X_2 - X'_2) < 0\} = \\ &\eta_{X_1, X_2} \end{aligned}$$

where in (6) and in (7) we used the continuity of the marginals  $F_{X_1}, F_{X_2}, F_U$ , in (7) we also used the fact that

$$(X_2 - X'_2)(X_3 - X'_3) \geq 0 \Rightarrow \text{either } X_i \geq X'_i, i = 2, 3 \text{ or } X_i < X'_i, i = 2, 3$$

so that  $F_{X_2, X_3}$  being monotonically non-decreasing implies  $(X_3 - X'_3)(U - U') \geq 0$ . Finally, in (8) we used the hypothesis (ii) in the proposition.

Analogously, we prove that  $\eta_{X_1, U} \geq \eta_{X_1, X_3}$  and the proposition is proved for  $n = 3$ . In the case  $n > 3$  the ideas are similar. For  $i, j \in \{2, 3, \dots, n\}, i \neq j$ , we have that

$$\begin{aligned} \eta_{X_1, U_2} &= P\{(X_1 - X'_1)(U_2 - U'_2) \geq 0\} = \\ &P\{(X_1 - X'_1)(X_i - X'_i)^2(U_2 - U'_2) \geq 0\} \geq \\ &P\{(X_1 - X'_1)(X_i - X'_i) \geq 0, (X_i - X'_i)(U_2 - U'_2) \geq 0\} = \\ &P\{(X_1 - X'_1)(X_i - X'_i) \geq 0, (X_i - X'_i)(X_j - X'_j)^2(U_2 - U'_2) \geq 0\} = \\ &P\{(X_1 - X'_1)(X_i - X'_i) \geq 0, (X_i - X'_i)(X_j - X'_j) \geq 0\} + \\ &P\{(X_1 - X'_1)(X_i - X'_i) \geq 0, (X_i - X'_i)(X_j - X'_j) < 0, \\ &\quad (X_j - X'_j)(U_2 - U'_2) < 0\} = \\ &P\{(X_1 - X'_1)(X_i - X'_i) \geq 0, (X_i - X'_i)(X_j - X'_j) \geq 0\} + \\ &P\{(X_1 - X'_1)(X_i - X'_i) \geq 0, (X_i - X'_i)(X_j - X'_j) < 0\} = \\ &P\{(X_1 - X'_1)(X_i - X'_i) \geq 0\} = \eta_{X_1, X_i} \end{aligned}$$

for  $2 \leq i \leq n$ , where in the last equality we used two things. First, the hypothesis (i) plus the monotonicity of  $F_{X_2, \dots, X_n}$  for the first term in the sum and second, the hypothesis (ii) plus the monotonicity of the joint distribution function in the second term. ■

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