LOWER BOUNDS ON MULTIVARIATE DISTRIBUTIONS WITH PREASSIGNED MARGINALS

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It is well known that the Fréchet lower bound on bivariate distributions with given marginals, F_1 and F_2 , given by

$$\max\left\{F_1(x_1)+F_2(x_2)-1,0\right\},\$$

cannot be extended for the case of three or more dimensions. To overcome this difficulty, in order to arrive at a sharp lower bound for multivariate distributions with preassigned marginals, we introduce the concept of the moment of inertia of a multivariate distribution about a given line in \mathbb{R}^n and construct the distribution with the maximal moment of inertia about the line corresponding to the lower Fréchet bound. The multinormal case is discussed in some detail.

1. Introduction

In this paper we suggest an *n*-variate extension to the Fréchet lower bound for bivariate cumulative distribution functions (c.d.f.s). Recall that for $\Pi(F_1, F_2)$, the class of bivariate c.d.f.s with marginals F_1 and F_2 , the Fréchet lower bound is defined as

$$H_*(x,y) = \max \{F_1(x) + F_2(y) - 1, 0\}$$

This does not lend itself to any straight-forward extension to the case of $\Pi(F_1, F_2, \ldots, F_n)$ when n > 2 where $\Pi(F_1, F_2, \ldots, F_n)$ is the class of all c.d.f.s whose univariate marginals are the c.d.f.s F_1, F_2, \ldots, F_n . However, by observing that the Fréchet upper bound for this class,

$$H^*(x_1, x_2, \ldots, x_n) = \min \{F_1(x_1), \ldots, F_n(x_n)\},\$$

concentrates all the density on the curve

$$\{(x_1,\ldots,x_n)|F_1(x_1)=\cdots=F_n(x_n)\},\$$

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we were led to seek, as a lower bound, a c.d.f. which maximized the moment of inertia about this curve.

In the sections that follow we define the Fréchet bounds and prove that the lower bound is not extendable to classes of *n*-variate c.d.f.s for n > 2. We then define the moment of inertia as a measure of dependence of *n*-variate c.d.f.s and use it to present an alternative lower bound for $\Pi(F_1, \ldots, F_n)$. We conclude with specific applications to the multinormal distribution.

2. Assumptions and Notation

In this paper, when referring to $\Pi(F_1, F_2, \ldots, F_n)$ we shall assume the univariate marginals are continuous.

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} dt$$
, the univariate standard normal c.d.f.

$$\Phi_{\mu,\sigma}(x) = rac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{x} e^{-rac{(t-\mu)^2}{2\sigma^2}} dt, ext{ the univariate } N(\mu,\sigma) ext{ c.d.f.}$$

3. Motivation

It was discovered by Hoeffding (1940) and later rediscovered by Fréchet (1951) that for any F and $G, \Pi(F,G)$ contains an upper bound and a lower bound. The upper bound is min $\{F(x), G(y)\}$, denoted by $H^*_{F,G}(x,y)$ while the lower bound is max $\{F(x) + G(y) - 1, 0\}$, denoted by $H_{*F,G}(x,y)$. That is, for any $H \in \Pi(F,G)$ and all $(x,y) \in \mathbb{R}^2$, $H_*(x,y) \leq H(x,y) \leq H^*(x,y)$.

For $n > 2, H^*(x_1, \ldots, x_n) = \min \{F_1(x_1), \ldots, F_n(x_n)\}$ is a valid extension of the bivariate Fréchet upper bound. That is, it is an element of $\Pi(F_1, \ldots, F_n)$ and an upper bound for this class. However, the corresponding *n*-dimensional extension of $H_*(x_1, \ldots, x_n) = \max \{1 - \sum_{i=1}^n (1 - F_i(x_i)), 0\}$ is not an element of $\Pi(F_1, \ldots, F_n)$ for n > 2. This was shown by Feron (1965) and Dall'Aglio (1960). Moreover, when H_* is not an element of $\Pi(F_1, \ldots, F_n)$, then it can be shown that this class contains no lower bound.

In fact, we have the well known

THEOREM 1 Let F_1, \ldots, F_n be continuous. Then $\Pi(F_1, \ldots, F_n)$ contains no lower bound.

This result led us to seek alternative concepts for defining an extension of H_* for n > 2. We examined other ways in which H_* is extreme and sought to

construct elements of $\Pi(F_1, \ldots, F_n)$ that share these qualities. The following lemmas are part of this pursuit.

4. Preliminary Results

While accepting that $\Pi(F_1, \ldots, F_n)$ contains no lower bound, insight about elements of this class with other extreme characteristics can be gained by observing properties such a bound would have were one to exist. We will then seek to construct distributions with such properties to observe whether they are in any sense extreme elements of $\Pi(F_1, F_2, \ldots, F_n)$.

LEMMA 1 Let F be a univariate c.d.f. A lower bound for $\Pi(F, F, \ldots, F)$ must be (finitely) exchangeable, i.e. invariant under permutations of its arguments.

PROOF Let $H_L(x)$ be a lower bound for $\Pi(F, \ldots, F)$. Let $\gamma(x)$ be a permutation of the components of \mathbf{x} , i.e. $\gamma : \mathbb{R}^n \frac{1-1}{onto} \mathbb{R}^n$ by $\gamma(x_1, \ldots, x_n) = (x_{i_1}, \ldots, x_{i_n})$ where $\{1, 2, \ldots, n\} = \{i_1, \ldots, i_n\}$. If $H_L(\mathbf{x})$ is not exchangeable, $\exists \gamma$ and \mathbf{x}_1 such that $H_L(\mathbf{x}_1) \neq H_L(\gamma(\mathbf{x}_1))$. Without loss of generality, let $H_L(\mathbf{x}_1) < H_L(\gamma(\mathbf{x}_1))$. Define $H'_L(\mathbf{x}) = H_L(\gamma^{-1}(\mathbf{x}))$. Since the marginals of H_L are all equal, $H'_L \in \Pi(F, F, \ldots, F)$. Also $H'_L(\gamma(\mathbf{x}_1)) = H_L\{\gamma^{-1}(\gamma(\mathbf{x}_1))\} = H_L(\mathbf{x}_1) < H_L(\gamma(\mathbf{x}_1))$ which contradicts the assumption that H_L is a lower bound for $\Pi(F, \ldots, F)$. \Box

5. The Moment of Inertia

We consider $H_{*F,G}$ as the distribution of extreme negative dependence. Intuitively, it is the distribution in $\Pi(F,G)$ giving the most probability to points, (x,y), for which x and y are far apart; i.e. points away from the diagonal $\{(x,y)|F(x) = G(y)\}$. Let d((a,b);F,G) denote the distance of a point (a,b) from the curve $\{(x,y)|F(x) = G(y)\}$; i.e.

$$d((a,b);F,G) = \inf_{(z,w)\in\{F(x)=G(y)\}} \left\{ \sqrt{(a-z)^2 + (b-w)^2} \right\}.$$

Let (A, B) be a random vector distributed according to $H \in \Pi(F, G)$. Then, d((A, B); F, G) is a random variable whose distribution is determined by H. The expected value, $E(d^2)$ which we shall label $\mu(H)$, can then be considered as a measure of (negative) dependence of H. Then, any $H_L \in$ $\Pi(F, G)$ for which μ is maximized could be considered a distribution of extreme negative dependence. EXAMPLE Let (X, Y) be uniformly distributed on $(0, 1)^2$, i.e., $H_{x,y}(x, y)$ has p.d.f.

$$f_{x,y}(x,y) = \left\{egin{array}{c} 1 ext{ for } (x,y) \in (0,1)^2 \ 0 ext{ otherwise} \end{array}
ight.$$

Since $F_x = F_y$, we may consider the moment of inertia about the line defined by x = y. Then, by definition

$$\mu(H) \equiv E_H \left\{ d^2\left((s,t); F_x, F_y\right) \right\} = \int_0^1 \int_0^1 \frac{(s-t)^2}{2} ds dt = \frac{1}{12}.$$

More generally,

DEFINITION For any $H \in \Pi(F_1, \ldots, F_n)$, the moment of inertia of H about the curve $\{\mathbf{x}|F_1(x_1) = \ldots = F_n(x_n)\}$ is the expected value, according to H, of d^2 , where d is the distance between points \mathbf{x} in \mathbb{R}^n and this curve.

As an example application of these concepts we shall deal with $\Pi(\Phi, \Phi, \ldots, \Phi)$, the class of standard multinormal distributions. A lower bound of $\Pi(\Phi, \ldots, \Phi)$ must be exhangeable, and its variance/covariance matrix must be of the form (a_{ij}) where $a_{ii} = 1, \forall i = 1, \ldots, n$ and $a_{ij} = a \forall i, j$ such that $i \neq j$. The upper bound for $\Pi(\Phi, \Phi, \ldots, \Phi)$ is $H^*(\mathbf{x}) = \min(\Phi(x_i), \ldots, \Phi(x_n))$ with density concentrated on the curve

$$\{ \mathbf{x} | \Phi(x_1) = \ldots = \Phi(x_n) \} = \{ \mathbf{x} | x_1 = \ldots = x_n \}$$

because Φ is continuous and strictly increasing. A further requirement for our lower bound should be that it maximize the moment of inertia about this line. Straightforward calculations show that this moment of inertia is:

$$\frac{1}{n}\sum_{i< j} \left[\sigma_{x_i}^2 + (E(x_i))^2 + \sigma_{x_j}^2 + (E(x_j))^2 - 2\operatorname{cov}(x_i, x_j) - 2E(x_i)E(x_j)\right]$$

With the covariance matrix (a_{ij}) , this moment becomes:

$$\frac{1}{n}\sum_{i< j} \left[1+0+1+0-2a-2(0)\right] = \frac{1}{n}\frac{n(n-1)}{2}2(1-a) = (n-1)(1-a)$$

To maximize it, we must thus minimize a.

REMARK 1 If $H_L(\mathbf{x})$ is a lower bound for $\Pi(\Phi, \ldots, \Phi)$, then it can be shown that its moment of inertia about the line $\{\mathbf{x}|x_1 = x_2 = \ldots = x_n\}$, denoted by $\mu(H_L)$, satisfies $\mu(H_L) \ge \mu(H) \forall H \in \Pi(\Phi, \ldots, \Phi)$. So if we find $H_M \in \Pi(\Phi, \ldots, \Phi)$ such that $\mu(H_M) \ge \mu(H) \forall H$ and there actually were an $H_L \in \Pi(\Phi, \ldots, \Phi)$ such that $H_L(\mathbf{x}) \le H_M(\mathbf{x}) \forall \mathbf{x}$, then $\mu(H_L) \ge \mu(H_M)$, and hence $\mu(H_L) = \mu(H_M)$. Namely, we may not have an actual lower bound of $\Pi(\Phi, \ldots, \Phi)$ using this procedure of maximization, but we will have a correct upper bound for $\mu(H)$.

LEMMA 2 The determinant of the $n \times n$ matrix, $A, (n \ge 2)$ whose diagonal elements are 1's and other elements are equal to some real number a is

$$(n-1)(a+\frac{1}{n-1})(1-a)^{n-1}$$

PROOF See, for example, Graybill (1969). \Box

REMARK 2 Since the covariance matrix for a multinormal distribution must have a positive determinant, and since here $|a| \leq 1$ in order that A be a legitimate variance-covariance matrix, we must have $a > -\frac{1}{n-1}$. Hence, $-\frac{1}{n-1}$ is the lower bound for a which yields:

$$\sup_{H \in \Pi(\Phi,...,\Phi)} \mu(H) = (n-1) \left(1 - (-\frac{1}{n-1}) \right) = n$$

The question arises, what multivariate distribution results in setting $a = -\frac{1}{n-1}$ in the covariance matrix of the form depicted above?

Since the determinant of:

$$\begin{pmatrix} 1 & -\frac{1}{n-1} & \dots & -\frac{1}{n-1} \\ -\frac{1}{n-1} & 1 & & \\ \vdots & & \ddots & \vdots \\ -\frac{1}{n-1} & \dots & & 1 \end{pmatrix}$$

is zero, the p.d.f. does not exist. We shall therefore write the p.d.f. in terms of a and observe the limiting distribution as $a \to -\frac{1}{n-1}$.

LEMMA 3 Let A be the matrix described in Lemma 2. Then $A^{-1} = (b_{ij})$ where $b_{ii} = -\frac{(n-2)a+1}{((n-1)a+1)(a-1)} \forall i = 1, 2, ..., n$, and $b_{ij} = \frac{a}{((n-1)a+1)(a-1)}$ for $i \neq j$.

PROOF See, for example, Graybill (1969). \Box

Applying Lemmas 2 and 3 and straightforward calculations yield the following expression for the p.d.f. in terms of a:

$$\frac{\sqrt{c}}{(2\pi)^{\frac{n}{2}}\sqrt{(n-1)(1-a)^{n-1}}} \times (1) \exp\left\{-\frac{c}{2(n-1)(1-a)}\left[((n-2)a+1)\sum_{j=1}^{n}x_{j}^{2}-2a\sum_{i< j}x_{i}x_{j}\right]\right\}$$

where $c = \frac{n-1}{a(n-1)+1}$. As $a \to -\frac{1}{n-1}$, the limit of the p.d.f. becomes

$$\lim_{c \to \infty} \frac{\sqrt{c}}{(2\pi)^{\frac{n}{2}} \sqrt{\frac{n^{n-1}}{(n-1)^{n-2}}}} \exp\left\{-\frac{c}{2n(n-1)} (\sum_{j=1}^n x_j)^2\right\}$$
$$= \begin{cases} 0 \text{ for all } \mathbf{x} \text{ such that } \sum_{j=i}^n x_j \neq 0\\ \infty \text{ for all } \mathbf{x} \text{ such that } \sum_{i=i}^n x_i = 0 \end{cases}$$

This result should have been expected. The "density" is concentrated totally on the hyperplane $(\mathbf{x}|\sum_{i=1}^{n} x_i = 0)$ perpendicular to the line $(\mathbf{x}|x_i = \ldots = x_n)$ containing $(0, \ldots, 0) = (E(x_1), \ldots, E(x_n))$.

Via direct computation, we can show that this concentration of density corresponds to a legitimate *n*-dimensional c.d.f. Labeling this c.d.f. $H_{-\frac{1}{n-1}}$, we see that $H_{-\frac{1}{n-1}}(\mathbf{t})$, is the value of the (n-1)-dimensional mass (density) contained in the (n-1)-dimensional simplex

$$\left\{\mathbf{x} \mid \sum_{i=1}^n x_i = 0\right\} \bigcap \left\{\mathbf{x} \mid x_1 \leq t_1, \ldots, x_n \leq t_n\right\}.$$

Integrating the p.d.f. (1), over this simplex, and taking the limit as $a \rightarrow -\frac{1}{n-1}$ yields

(2)
$$\frac{1}{(2\pi)^{\frac{n-1}{2}}\sqrt{|A|}}\exp\left\{-\frac{1}{2}(x_2,\ldots,x_n)A^{-1}(x_2\ldots,x_n)'\right\}$$

where A is now the $(n-1) \times (n-1)$ matrix whose elements

$$a_{ij} = \begin{cases} 1 & i = j \\ -\frac{1}{n-1} & i \neq j \end{cases}$$

and whose determinant is (cf Lemma 2) $\frac{n^{n-2}}{(n-1)^{n-1}}$.

The result (2) was intuitively expected. The limiting density does exist and is obtained by placing an (n-1)-dimensional normal density in the (n-1)-dimensional hyperplane $\{\mathbf{x}|\sum_{i=1}^{n} x_i = 0\}$.

An alternative approach to this analysis involves the application of multivariate characteristic functions and the Lévy-Cramér continuity theorem.

EXAMPLES

Case n = 2. In this case the hyperplane becomes $\{(x, y) | x + y = 0\}$ or the line y = -x. The value of this density at (x, -x) by (2) is $\frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}$, and

the corresponding $H_L(x,y)$ is derived by noting that for all (x,y) such that $x+y \leq 0$, $H_L(x,y) = 0$, and for (x,y) such that x+y > 0, we must calculate the mass contained on the line segment between (-y,y) and (x,-x). In other words, here $H_L(x,y) = \frac{1}{\sqrt{2\pi}} \int_{-y}^x e^{-\frac{t^2}{2}} dt = \Phi(x) - \Phi(-y) = \Phi(x) + \Phi(y) - 1$. Thus, in this case $H_L(x,y) = \max \{ \Phi(x) + \Phi(y) - 1, 0 \}$ which is the lower Fréchet bound for $\Pi(\Phi, \Phi)$.

Case n = 3. Note that here $H_L(x, y, z)$ is concentrated on the plane $\{(x, y, z) | x + y + z = 0\}$. Analogous but somewhat more involved calculations yield "the lower bound" of the form

$$H_L(u, v, w) = \max\left\{\int_{-(u+w)}^{v} e^{-\frac{y^2}{2}} \left[\Phi(\frac{y+2w}{\sqrt{3}}) + \Phi(\frac{y+2u}{\sqrt{3}}) - 1\right] dy, 0\right\}$$

The calculation of $H_L(u, v, w)$ involves computation of the probability mass in the set

$$\{(x, y, z) | x \le u, y \le v, z \le w\} \bigcap \{(x, y, z) | x + y + z = 0\}.$$

(Details are available from the authors upon request.)

Finally, we note that if $H_L(\mathbf{x})$ is a lower bound for all *n*-dimensional standard multinormal c.d.f.s, then $H'_L(\mathbf{x}) \equiv H_L\left\{\frac{x_1-\mu_1}{\sigma_1}, \ldots, \frac{x_n-\mu_n}{\sigma_n}\right\}$ is a lower bound for all multinormal *n*-dimensional c.d.f.s in $\Pi(\Phi_{\mu_1,\sigma_1},\ldots,\Phi_{\mu_n,\sigma_n})$.

It is also straightforward to calculate that the corresponding upper bound on moment of inertia $\mu(H)$ in this case, denoted by $M_{H_{L'}}$, is

$$M_{H_L'} = \frac{2n}{(n-1)\sum \sigma_i^2} \sum_{i < j} \sigma_i^2 \sigma_j^2$$

which coincides for $\sigma_i^2 = 1, i = 1, \ldots, n$ with

$$\sup_{H \in \Pi(\Phi,...\Phi)} \mu(H) = n$$

CONCLUDING REMARK The approach suggested in this paper could be extended rather straightforwardly to other families of distributions. Of special interest may be the multivariate extensions of the Gumbel bivariate distribution (Gumbel (1960)) as well as other multivariate distributions with exponential or, more generally, Weibull marginals.

References

- DALL'AGLIO, G. (1960). Les Fonctions Extrêmes de la Classes de Fréchet à Trois Dimensions. Publ. Inst. Stat. Univ. Paris 9 175-188.
- FERON, R. (1965). Sur les Tableaux de Corrélation dont les Marges sont Données, cas de l'espace à Trois Dimensions. Publ. Inst. Stat. Univ., Paris 5 3-12.
- FRÉCHET, M. (1951). Sur les Tableaux de Corrélation dont les Marges sont Données. Ann. Univ. Lyon, Sect. A 14 53-77.
- GRAYBILL, F. A. (1969). Introduction to Matrices with Applications in Statistics. 1st edition. Wadsworth, Belmont, CA.
- GUMBEL, E. J. (1960). Bivariate Exponential Distributions. J. Amer. Stat. Assoc. 55 698-707.
- HOEFFDING, W. (1940). Masstabinvariante Korrelationstheorie. In Schriften des mathematischen Instituts und des Instituts f
 ür Angewandte Mathematik der Universitat. Berlin 5 179-233.
- MARDIA, K. V. (1970). Families of Bivariate Distributions. Hafner, Darien, CT.
- NATAF, A. (1962). Détermination des Distributions de Probabilitiés dont les Marges sont Données. Comptes Rendus de l'Académie des Sciences 255 Paris, 42-43.
- SKLAR, A. (1973). Random Variables, Joint Distribution Functions, and Copulas. *Kybernetica* 9 449-460.

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