EXTREME POINTS OF THE N-DIMENSIONAL ELLIPTOPE:

APPLICATION TO UNIVERSAL COPULAS

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Abstract

Based on the explicit parameterization of the set of positive semi-definite correlation matrices, we derive simple spherical coordinates for their extreme points. An application to the construction of universal copulas is included.

Keywords

correlation matrix, positive semi-definite property, canonical parameterization, extreme points, universal copula, linear circular copula

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1. Introduction

A positive semi-definite matrix whose diagonal entries are equal to one is called a *correlation matrix*. The compact convex set of *nxn* correlation matrices $(r_{ij}), 1 \le i, j \le n$, is called *elliptope* (for **ellip**soid and poly**tope**), a terminology coined by Laurent and Poljak (1995). The study of the elliptope structure has generated many interesting and partly difficult problems. For example, the extreme points of the elliptope have not been explicitly determined, though the rank one and two extreme points are known and there exist characterization results on them by Ycart (1985), Li and Tam (1994), and Parthasarathy (2002).

Clearly, the elliptope is uniquely determined by the set of $\frac{1}{2}(n-1)n$ upper diagonal elements $r = (r_{ij}), 1 \le i < j \le n$, denoted by E_n. Hürlimann (2014a), Theorem 3.1, constructs an explicit parameterization of the correlation matrix, which maps bijectively any $x = (x_{ij}) \in [-1,1]^{\frac{1}{2}(n-1)n}$ to

$r=(r_{ij})\in E_n$. These so-called Cartesian coordinates depend very simply on x_{ij}, as well as on products $x_{ij}x_{k\ell}$ and sums of products, which additionally involve the functional quantities

$$y_{ij,\ell}=y_{ij,\ell}(x_{i\ell},x_{j\ell})=\sqrt{(1-x_{i\ell}^2)(1-x_{j\ell}^2)}\,. \tag{1.1}$$

The notation (1.1) will be used throughout without further mention of its definition.

The required preliminary results are summarized in Section 2. Combining the relatively simple characterization of the extreme points of correlation matrices by Ycart (1985) with our Cartesian coordinates, a fully explicit functional parameterization of the extreme points is derived in Section 3. It should be most useful in problems depending on the knowledge of extreme points of correlation matrices. We illustrate with an application to the construction of some universal n-copulas, a problem which remains unsolved in general (e.g. Devroye and Letac (2010), Hürlimann (2014b), Letac (2014)).

2. Preliminary results

There are two questions related to extreme points of the elliptope, namely the existence of extreme points and their construction. The existence question depends upon the rank of a correlation matrix and has been settled by many authors (e.g. Ycart (1985), Proposition 6, Grone et al. (1990), Theorem 2, Li and Tam (1994), Corollary 2, Parthasarathy (2002), Corollary 2.2). For infinite dimensional correlation matrices the question is considered in Kiukas and Pellonpaa (2008). Some earlier work on extreme points in convex sets of symmetric and Hermitian matrices includes Christensen and Verterstrom (1979) and Loewy (1980).

Theorem 2.1 (*Existence of extreme points*). There exist extreme points of rank m if, and only if, the dimension of the elliptope satisfies the inequality $n\geq\frac{1}{2}m(m+1)$.

Up to now the effective construction of all extreme points has been an open problem. Different characterization conditions for them have been obtained by Ycart (1985), Theorem 2, Li and Tam (1994), Theorem 1 (b), and Parthasarathy (2002), Theorem 2.1. The characterization by Ycart (1985) is most appropriate to the present needs.

Theorem 2.2 (*Ycart's characterization of extreme points*). A nxn correlation matrix $(r_{ij})\in E_n, 1\leq i<j\leq n$, of rank m, such that $n\geq\frac{1}{2}m(m+1)$, is an extreme point if, and only if, there exist $a_{is}\in[-1,1],\ i=1,...,n,\ s=1,...,m$, which solve the quadratic system of equations

$$r_{ij}=\sum_{s=1}^{m}a_{is}a_{js},\ 1\leq i<j\leq n,\quad \sum_{s=1}^{m}a_{is}^2=1,\ i=1,...,n\,. \tag{2.1}$$

In Section 3 we combine Ycart's characterization with the following so-called canonical parameterization to obtain a parameterization of the extreme points.

Theorem 2.3 (*Cartesian coordinates of n-dimensional elliptope*). There exists a bijective mapping between the cube $[-1,1]^{\frac{1}{2}(n-1)n}$ and E_n, which maps the Cartesian coordinates $x=(x_{ij})$ to $r=(r_{ij})$ such that

$$r_{in}=x_{in},\quad i=1,...,n-1,\quad n\geq 2, \tag{2.2}$$

$$r_{in-1}=x_{in}x_{n-1n}+x_{in-1}y_{in-1,n},\quad i=1,...,n-2,\quad n\geq 3, \tag{2.3}$$

$$r_{in-k}=x_{in}x_{n-kn}+\sum_{j=2}^{k}x_{in-j+1}x_{n-kn-j+1}\prod_{\ell=n-j+2}^{n}y_{in-k,\ell}+x_{in-k}\prod_{\ell=n-k+1}^{n}y_{in-k,\ell}, \tag{2.4}$$
$$i=1,...,n-k-1,\quad k=2,...,n-2,\quad n\geq 4$$

Proof. Consult Hürlimann (2014a), Theorem 3.1. ◊

3. Extreme points of correlation matrices

Our main result is the following canonical parameterization of the extreme points in the convex compact set of all correlation matrices.

Theorem 3.1 (*Extreme points of n-dimensional elliptope*). Let $r=(r_{ij})\in E_n$ be an extreme point of $rank(r)=m\geq 1,\ n\geq \max\{2,\frac{1}{2}m(m+1)\}$ in canonical form (2.2)-(2.4). Then, there exist spherical coordinates $\alpha_{ik}\in[0,\pi],\quad k=1,...,m-1,\ i=1,...,n-k,$ such that

Case 1: $rank(r)=1,\quad n\geq 2$

$$r_{in}=\varepsilon_i\in\{-1,1\},\quad i=1,...,n-1,\quad r_{in-k}=\varepsilon_i\varepsilon_{n-k},\quad k=1,...,n-2,\ i=1,...,n-k-1 \tag{3.1}$$

Case 2: $rank(r)=2,\quad n\geq 3$

$$r_{in}=\cos\alpha_{i1},\quad i=1,...,n-1, \tag{3.2}$$

$$r_{in-k}=\cos(\alpha_{i1}-\alpha_{n-k1}),\quad k=1,...,n-2,\ i=1,...,n-k-1 \tag{3.3}$$

Case 3: $rank(r)=m\geq 3,\quad n\geq \frac{1}{2}m(m+1)$

$$r_{in}=\cos\alpha_{i1},\quad i=1,...,n-1, \tag{3.4}$$

$$r_{in-1}=\cos\alpha_{i1}\cos\alpha_{n-11}+\cos\alpha_{i2}\cdot\sin\alpha_{i1}\sin\alpha_{n-11},\quad i=1,...,n-2, \tag{3.5}$$

$$r_{in-k}=\cos\alpha_{i1}\cos\alpha_{n-k1}+\sum_{j=1}^{k-1}\cos\alpha_{ij+1}\cos\alpha_{n-kj+1}\cdot\prod_{s=1}^{j}\sin\alpha_{is}\sin\alpha_{n-ks} \tag{3.6}$$
$$+\cos\alpha_{ik+1}\cdot\prod_{s=1}^{k}\sin\alpha_{is}\sin\alpha_{n-ks},\quad i=1,...,n-k-1,\quad k=2,...,m-2$$

$$r_{in-k} = \cos\alpha_{i1}\cos\alpha_{n-k1} + \sum_{j=1}^{m-3}\cos\alpha_{ij+1}\cos\alpha_{n-kj+1}\cdot\prod_{s=1}^{j}\sin\alpha_{is}\sin\alpha_{n-ks}$$
$$+\cos(\alpha_{im-1}-\alpha_{n-km-1})\cdot\prod_{s=1}^{m-2}\sin\alpha_{is}\sin\alpha_{n-ks},\quad i=1,...,n-k-1,\quad k=m-1,...,n-2 \tag{3.7}$$

<u>Proof</u>. Case 1 is shown by many authors (e.g. Ycart (1985), Remark, p. 610, Laurent and Poljak (1995), Theorem 2.5, Parthasarathy (2002), Remark 2.4, p. 178). For $rank(r) = m \geq 2$ the idea is to express Ycart's equations (2.1) in spherical coordinates and make them consistent with the canonical form (2.2)-(2.4). Consider first Case 2. Using polar coordinates for the 1-sphere in R^2 one solves the second equations in (2.1) setting

$$a_{i1} = \cos\varphi_i,\quad a_{i2} = \sin\varphi_i,\quad i=1,...,n.$$

Inserted into the first equations of (2.1) one sees that

$$r_{ij} = a_{i1}a_{j1} + a_{i2}a_{j2} = \cos(\varphi_i - \varphi_j),\quad 1 \leq i < j \leq n. \tag{3.8}$$

On the other hand, in accordance with (2.2), there exists $\alpha_{i1} \in [0,\pi], i=1,...,n-1$, such that $r_{in} = x_{in} = \cos\alpha_{i1}$. Setting $j = n$ in (3.8) one has $r_{in} = \cos(\varphi_i - \varphi_n),\ i=1,...,n-1$. This matches the canonical parameterization $r_{in} = \cos\alpha_{i1}$ if one sets $\varphi_n = 0, \varphi_i = \alpha_{i1}, i=1,...,n-1$. The remaining equations in (3.8) read

$$r_{ij} = \cos(\alpha_{i1} - \alpha_{j1}),\quad 1 \leq i < j < n. \tag{3.9}$$

One must show that (3.9) matches exactly (2.3)-(2.4). From (2.3) one gets

$$r_{in-1} = x_{in}x_{n-1n} + x_{in-1}y_{in-1,n} = \cos\alpha_{i1}\cos\alpha_{n-11} + x_{in-1}\cdot\sin\alpha_{i1}\sin\alpha_{n-11},\quad i=1,...,n-2.$$

This matches $r_{in-1} = \cos(\alpha_{i1} - \alpha_{n-11})$ from (3.9) if, and only if, one has $x_{in-1} = 1$. Using this and Definition (1.1) one sees that

$$y_{in-k,n-1} = \sqrt{(1-x_{in-1}^2)(1-x_{n-kn-1}^2)} = 0,\quad k=2,...,n-2,\quad i=1,...,n-k-1.$$

Inserting into (2.4) one obtains (3.3) for $k=2,...,n-2, i=1,...,n-k-1$, and Case 2 is shown. To show Case 3 we distinguish between $m=3$ and $m \geq 4$. First, let $m=3$. Solve the second equations in (2.1) using spherical coordinates for the 2-sphere in R^3 such that

$$a_{i1} = \cos\varphi_i,\quad a_{i2} = \sin\varphi_i\cos\vartheta_i,\quad a_{i3} = \sin\varphi_i\sin\vartheta_i.$$

Inserting into the first equations of (2.1) one obtains

$$r_{ij}=\sum_{s=1}^{3}a_{is}a_{js}=\cos\varphi_i\cos\varphi_j+\sin\varphi_i\sin\varphi_j\cdot\cos(\vartheta_i-\vartheta_j),\quad 1\le i<j\le n. \qquad (3.10)$$

In particular, one has $r_{in}=\cos\varphi_i\cos\varphi_n+\sin\varphi_i\sin\varphi_n\cdot\cos(\vartheta_i-\vartheta_n),\quad i=1,...,n-1$. On the other hand, in virtue of (2.2) one can set $r_{in}=x_{in}=\cos\alpha_{i1}$ for $\alpha_{i1}\in[0,\pi],\ i=1,...,n-1$. This matches the preceding expression if one sets $\varphi_n=0,\ \varphi_i=\alpha_{i1},\ i=1,...,n-1$. The remaining equations in (3.10) read

$$r_{ij}=\cos\alpha_{i1}\cos\alpha_{j1}+\sin\alpha_{i1}\sin\alpha_{j1}\cdot\cos(\vartheta_i-\vartheta_j),\quad 1\le i<j<n. \qquad (3.11)$$

From (2.3) one has $r_{in-1}=x_{in}x_{n-1n}+x_{in-1}y_{in-1,n}=\cos\alpha_{i1}\cos\alpha_{n-11}+x_{in-1}\cdot\sin\alpha_{i1}\sin\alpha_{n-11}$, with $x_{in-1}=\cos\alpha_{i2}$ for some $\alpha_{i2}\in[0,\pi],\ i=1,...,n-2$. This matches r_{in-1} in (3.11) if one sets $\vartheta_{n-1}=0,\ \vartheta_i=\alpha_{i2},\ i=1,...,n-2$. Then, the remaining equations in (3.11) read

$$r_{ij}=\cos\alpha_{i1}\cos\alpha_{j1}+\sin\alpha_{i1}\sin\alpha_{j1}\cdot\cos(\alpha_{i2}-\alpha_{j2}),\quad 1\le i<j<n-1. \qquad (3.12)$$

One must show that this matches exactly (2.4). For $i=1,...,n-3$ one obtains

$$\begin{aligned}r_{in-2}&=x_{in}x_{n-2n}+x_{in-1}x_{n-2n-1}y_{in-2,n}+x_{in-2}y_{in-2,n-1}y_{in-2,n}\\&=\cos\alpha_{i1}\cos\alpha_{n-21}+\sin\alpha_{i1}\sin\alpha_{n-21}\cdot\{\cos\alpha_{i2}\cos\alpha_{n-22}+x_{in-2}\cdot\sin\alpha_{i2}\sin\alpha_{n-22}\},\end{aligned}$$

which matches the corresponding entry in (3.12) if, and only if, one has $x_{in-2}=1$, which shows (3.7) for $k=2$ (of course (3.6) is a void statement here). Further, this implies that

$$y_{in-k,n-2}=\sqrt{(1-x_{in-2}^2)(1-x_{n-kn-2}^2)}=0,\quad k=3,...,n-2,\quad i=1,...,n-k-1.$$

Inserting into (2.4) one obtains (taking into account the vanishing components) the remaining formulas in (3.7) for $k=3,...,n-2$. It remains to generalize the preceding steps for a fixed rank $m\ge 4$. Using spherical coordinates for the $(m-1)$-sphere in R^m one solves the second equations in (2.1) setting

$$\begin{aligned}&a_{i1}=\cos\varphi_{i1},\quad a_{i2}=\sin\varphi_{i1}\cos\varphi_{i2},\quad a_{i3}=\sin\varphi_{i1}\sin\varphi_{i2}\cos\varphi_{i3},\quad ...,\\&a_{im-1}=\sin\varphi_{i1}\sin\varphi_{i2}...\sin\varphi_{im-2}\cos\varphi_{im-1},\quad a_{im}=\sin\varphi_{i1}\sin\varphi_{i2}...\sin\varphi_{im-2}\sin\varphi_{im-1}.\end{aligned}$$

Inserted into the first equations in (2.1) one obtains

$$\begin{aligned}r_{ij}&=\cos\varphi_{i1}\cos\varphi_{j1}+\sum_{\ell=1}^{m-3}\cos\alpha_{i\ell+1}\cos\alpha_{j\ell+1}\cdot\prod_{s=1}^{\ell}\sin\varphi_{is}\sin\varphi_{js}\\&+\cos(\varphi_{im-1}-\varphi_{jm-1})\cdot\prod_{s=1}^{m-2}\sin\varphi_{is}\sin\varphi_{js},\quad 1\le i<j\le n.\end{aligned} \qquad (3.13)$$

In virtue of (2.2) set $r_{in} = x_{in} = \cos\alpha_{i1}$ for $\alpha_{i1} \in [0,\pi], i = 1,...,n-1$. This matches the corresponding expression for r_{in} in (3.13) if one sets $\varphi_{n1} = 0, \varphi_{i1} = \alpha_{i1}, i = 1,...,n-1$. The formula (3.4) is shown. From (2.3) one gets

$$r_{in-1} = x_{in}x_{n-1n} + x_{in-1}y_{in-1,n} = \cos\alpha_{i1}\cos\alpha_{n-11} + x_{in-1}\cdot\sin\alpha_{i1}\sin\alpha_{n-11},$$

with $x_{in-1} = \cos\alpha_{i2}$ for some $\alpha_{i2} \in [0,\pi], i = 1,...,n-2$. This matches the expression for r_{in-1} in (3.13) if one sets $\varphi_{n-12} = 0, \varphi_{i2} = \alpha_{i2}, i = 1,...,n-2$. The formula (3.5) follows. Proceeding in the same manner, one obtains from (2.4) for $k = 2,...,m-2, i = 1,...,n-k-1,$ the expressions

$$\begin{aligned} r_{in-k} &= x_{in}x_{n-kn} + \sum_{j=2}^{k} x_{in-j+1}x_{n-kn-j+1}\prod_{\ell=n-j+2}^{n} y_{in-k,\ell} + x_{in-k}\prod_{\ell=n-k+1}^{n} y_{in-k,\ell} \\ &= \cos\alpha_{i1}\cos\alpha_{n-k1} + \sum_{j=1}^{k-1}\cos\alpha_{ij+1}\cos\alpha_{n-kj+1}\cdot\prod_{s=1}^{j}\sin\alpha_{is}\sin\alpha_{n-ks} + \cos\alpha_{ik+1}\cdot\prod_{s=1}^{k}\sin\alpha_{is}\sin\alpha_{n-ks}, \end{aligned}$$

where the fact that $x_{in-k} = \cos\alpha_{ik+1}$ for some $\alpha_{ik+1} \in [0,\pi], i = 1,...,n-k+1$, has been used. This choice matches the corresponding equations for r_{in-k} in (3.13) if one sets $\varphi_{n-kk+1} = 0, \varphi_{ik+1} = \alpha_{ik+1}, k = 2,...,m-2, i = 1,...,n-k-1$. This shows the formula (3.6). It remains to show that the remaining equations in (3.13) for r_{ij} with $1 \le i < j < n-m+2$ match exactly the corresponding expressions in (2.4). First, one has

$$\begin{aligned} r_{in-m+1} &= x_{in}x_{n-m+1n} + \sum_{j=2}^{m-1} x_{in-j+1}x_{n-m+1n-j+1}\prod_{\ell=n-j+2}^{n} y_{in-m+1,\ell} + x_{in-m+1}\prod_{\ell=n-m+2}^{n} y_{in-m+1,\ell} \\ &= \cos\alpha_{i1}\cos\alpha_{n-m+11} + \sum_{j=1}^{m-3}\cos\alpha_{ij+1}\cos\alpha_{n-m+1j+1}\cdot\prod_{s=1}^{j}\sin\alpha_{is}\sin\alpha_{n-m+1s} \\ &+ \{\cos\alpha_{im-1}\cos\alpha_{n-m+1m-1} + x_{in-m+1}\cdot\sin\alpha_{im-1}\sin\alpha_{n-m+1m-1}\}\cdot\prod_{s=1}^{m-2}\sin\alpha_{is}\sin\alpha_{n-m+1s}. \end{aligned}$$

This matches the corresponding expression in (3.13) if, and only if, one has $x_{in-m+1} = 1$, which shows (3.7) for $k = m-1$. Further, this implies that

$$y_{in-k,n-m+1} = \sqrt{(1-x_{in-m+1}^2)(1-x_{n-kn-m+1}^2)} = 0, \quad k = m,...,n-2, \quad i = 1,...,n-k-1.$$

Inserting into (2.4) for $k = m,...,n-2, \quad i = 1,...,n-k-1$, one obtains similarly to the above the remaining formulas in (3.7). Theorem 3.1 is shown. ◊

Remarks 3.1. Case 2 has also been solved by Ycart (1985), Corollary, p. 611. In Cases 2 and 3 one must ensure that the correlation matrices are of rank m. This is fulfilled provided the vectors

$a_i^T = (a_{1i}, a_{2i}, ..., a_{ni}), i = 1,...,m$, defined in the proof of Theorem 3.1, are linearly independent. It is well-known that this holds if, and only if, the determinant of the Gram matrix $G_{ij} = (< a_i, a_j >)$ is non-zero. This is always satisfied up to some degenerate cases. For example, if $m = 2$, it suffices that $\alpha_i \neq 0, \pi$ for some index $i \in \{1,..., n-1\}$.

4. Application to the construction of universal copulas

A n-dimensional copula is called *n-universal* if every n-dimensional valid correlation matrix can be realized as a rank correlation matrix, i.e. there exists a n-variate uniform distribution with this rank correlation structure. In the literature 2-universal copulas are better known under the naming comprehensive or inclusive copulas (see e.g. Nelsen (2006)). Although the existence of 3-universal copulas has been settled by several authors (e.g. Joe (1997), Exercise 4.17, pp. 137-138, Kurowicka and Cooke (2006), Section 4.4.6, p.102, Devroye and Letac (2010)), the effective construction of 3-universal copulas is more difficult. Hürlimann (2014d) constructs an analytical 3-universal copula that is based on the bivariate linear circular copula in Perlman and Wellner (2011). The latter copula seems to have been independently obtained by Kurowicka et al. (2000), which called it „elliptical copula". As pointed out by Letac (2014), the linear circula copula is a special case of probability distributions studied by Gasper (1971). This 2-universal copula can be used to construct n-universal copulas for rank two extremal correlation matrices. Reduced to its essential steps, the presentation by Letac (2014) has an elementary appeal.

Let $B_2 \subset R^2$ be the unit disk and $C_2 = [-1,1]^2$ the centered square. Consider the linear circular copula density with uniform [-1,1] margins U, V defined by

$$p_{(U,V)}(u,v) = \begin{cases} \dfrac{1}{2\pi\sqrt{1-u^2-v^2}}, & (u,v) \in B_2, \\ 0, & (u,v) \in C_2 - B_2. \end{cases} \tag{4.1}$$

A crucial step towards the main result below is the following elementary result.

Lemma 4.1 (*n-universal rank two extreme linear circular copula*) Given is the extreme correlation matrix of rank two of the form

$$r = (r_{ij}) = (\cos(\alpha_i - \alpha_j)), \quad \alpha_i \in [0, 2\pi], 1 \le i, j \le n.$$

Then, there exist a random vector $(X_1, X_2, ..., X_n)$ with uniform [-1,1] margins $X_i, i = 1,...,n$, and rank two correlation matrix $r = (r_{ij})$.

Proof. Consider the random vector $(X_1, X_2, ..., X_n)$ defined by

$$X_i = \cos(\alpha_i) \cdot U + \sin(\alpha_i) \cdot V, \quad i = 1,...,n,$$

where the random pair (U,V) has the linear circular copula density (4.1). Clearly, the variables $X_i, i=1,...,n$, are uniform [-1,1] random variables. Moreover, through application of the Jacobian transformation method, one sees that the probability density of $(X_i, X_j), 1 \le i \le j \le n$, is given by

$$p_{(X_i,X_j)}(x,y) = \begin{cases} \dfrac{1}{2\pi\sqrt{(1-r_{ij}^2)(1-x^2)-(y-r_{ij}x)^2}}, & (x,y)\in E_{r_{ij}}, \\ 0, \quad (u,v)\in C_2 - E_{r_{ij}}, & \end{cases} \tag{4.2}$$

where the support $E_{r_{ij}} = \left\{(x,y) \,\middle|\, x^2+y^2-2r_{ij}xy < 1-r_{ij}^2\right\}$ is the inner of an ellipse, and $r_{ij} = \cos(\alpha_i - \alpha_j)$ coincides with the correlation coefficient of the pair (X_i, X_j) (e.g. Kurowicka et al. (2000), Perlman and Wellner (2011), Hürlimann (2014d), Section 3). ◊

Theorem 4.1 (n *-universal rank two copula*) Given is a rank two correlation matrix $r=(r_{ij}), 1 \le i, j \le n$. Then, there exist a random vector $(X_1, X_2, ..., X_n)$ with uniform [-1,1] margins $X_i, i=1,...,n$, and rank two correlation matrix $r=(r_{ij})$.

Proof. This follows through application of the theorem of Carathéodory (1911) and Steinitz (1914). Any valid correlation matrix (of rank two) is a finite convex combination of extreme correlation matrices (of rank two). Since the result holds for the extreme correlation matrices of rank two by Lemma 4.1, the result follows. ◊

One notes that Theorem 4.1 settles the existence question for n-universal copulas, $n=3,4,5$. Indeed, correlation matrices of dimensions $n=3,4,5$ have maximum rank two by Theorem 2.1.

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