Theoretical Mathematics & Applications, vol.4, no.3, 2014, 1-17
ISSN: 1792- 9687 (print), 1792-9709 (online)
Scienpress Ltd, 2014

Cartesian and Polar Coordinates for the N-Dimensional Elliptope

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Abstract

Based on explicit recursive closed form correlation bounds for positive semi-definite correlation matrices, we derive simple Cartesian and polar coordinates for them.

Mathematics Subject Classification: 15A24; 15B99; 62H20; 65F30
Keywords: Correlation matrix; Partial correlation; Positive semi-definite matrix; Determinantal identity; Recursive algorithm; Canonical parameterization

1 Introduction

The algorithmic generation of valid (i.e. positive semi-definite) correlation matrices is an interesting problem with many applications. The author derives in [4], Theorem 3.1, explicit recursively defined generic closed form correlation

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Article Info: *Received:* May 2, 2014. *Revised:* June14, 2014.
Published online : August 31, 2014.

bounds. Based on a new and more appropriate variant of this result, we construct simple Cartesian and polar coordinates for the space of all valid correlation matrices.

A positive semi-definite matrix whose diagonal entries are equal to one is called a correlation matrix. The convex set of nxn correlation matrices $R=(r_{ij}), 1 \le i, j \le n$, is called *elliptope* (stands for **ellip**soid and poly**tope**), a terminology coined by Laurent and Poljak [5]. It is a particular instance of a *spectrahedron*, whose study is at the interface between optimization, convexity, real algebraic geometry, statistics and combinatorics (see Vinzant [8]). 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. In the main Theorem 3.1, we construct an explicit parameterization of the elliptope, 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.

2 Determinantal identities for correlations and partial correlations

For fixed $n \ge 2$ let $R=(r_{ij}), 1 \le i, j \le n$ be an nxn correlation matrix. For each $m \in \{2,...,n\}$ and any index set $s^{(m)} = (s_1, s_2, ..., s_m)$ with $1 \le s_i \le n, i = 1,...,m$, consider the mxm sub-correlation matrix

$$R^{(m)} = (r_{s_i s_j}), 1 \le i, j \le m ,$$

which is uniquely determined by

$$r^{(m)} = (r_{s_i s_j}), 1 \le i < j \le m .$$

It is convenient to use own notations.

Definitions 2.1 (*Determinant, partial correlation and d-scaled partial correlation*)
The *determinant* of the matrix $R^{(m)}$ is denoted by

$$\Delta^m(s^{(m)}) = \Delta^m(s_1, s_2, ..., s_m) = \det(R^{(m)}) . \tag{2.1}$$

For $n \ge m \ge 3$ and an index set $s^{(m)}$ the *partial correlation* of (s_1, s_2) with respect to $(s_3, ..., s_m)$ is recursively defined and denoted by

$$r_{s_1 s_2; s_3,...,s_m} = \frac{r_{s_1 s_2; s_3,...,s_{m-1}} - r_{s_1 s_m; s_3,...,s_{m-1}} \cdot r_{s_2 s_m; s_3,...,s_{m-1}}}{\sqrt{(1 - r^2_{s_1 s_m; s_3,...,s_{m-1}}) \cdot (1 - r^2_{s_2 s_m; s_3,...,s_{m-1}})}} , \tag{2.2}$$

where for $m = 2$ the quantities used on the right hand side of (2.2) are by convention the correlations $r_{s_1 s_2}, r_{s_1 s_m}, r_{s_2 s_m}$. The transformed partial correlation defined and denoted by

$$\begin{aligned} N^m(s^{(m)}) &= N^m(s_1, s_2; ..., s_m) \\ &= r_{s_1 s_2; s_3,...,s_m} \cdot \sqrt{\Delta^{m-1}(s_1, s_3, ..., s_m) \cdot \Delta^{m-1}(s_2, s_3, ..., s_m)} \end{aligned} \tag{2.3}$$

is called *d-scaled* (determinant scaled) *partial correlation*, with $N^2(s_1, s_2) = r_{s_1 s_2}$.

Recall the product representation (e.g. Hürlimann [3], formula (2.10))

$$\begin{aligned} &\Delta^n(1,2,...,n) \\ &= \prod_{i=1}^{n-1}\left(1 - r^2_{in}\right) \cdot \prod_{i=1}^{n-2}\left(1 - r^2_{in-1;n}\right) \cdot \prod_{i=1}^{n-3}\left(1 - r^2_{in-2;n-1,n}\right) \cdot \prod_{k=3}^{n-2}\left\{\prod_{i=1}^{n-k-1}\left(1 - r^2_{in-k;n-k+1,...,n}\right)\right\} , \end{aligned} \tag{2.4}$$

where an empty product is set equal to one. We need a new variant of Proposition 2.1 in Hürlimann [4], which by the way must be corrected for misprints.

Proposition 2.1 (*Recursive relation for d-scaled partial correlations*) For all $i=1,...,n-k, \quad k=4,...,n-1, \quad n\geq 5$, one has the identity

$$\begin{aligned}&N^k(i,n-k+1;n-k+3,...,n)\cdot\Delta^{k-3}(n-k+4,...,n)\\&=N^{k-1}(i,n-k+1;n-k+4,...,n)\cdot\Delta^{k-2}(n-k+3,...,n)\\&-\left\{\begin{array}{l}N^{k-1}(i,n-k+3;n-k+4,...,n)\\ \cdot N^{k-1}(n-k+1,n-k+3;n-k+4,...,n)\end{array}\right\}.\end{aligned}\tag{2.5}$$

Proof This is shown by induction. For $k=4$ one has by the defining recursion (2.2) that

$$r_{in-3;n-1,n}=\frac{r_{in-3;n}-r_{in-1;n}\cdot r_{n-3n-1;n}}{\sqrt{(1-r_{in-1;n}^2)\cdot((1-r_{n-3n-1;n}^2))}}\text{, with}$$

$$r_{sn-1;n}=\frac{N^3(s,n-1;n)}{\sqrt{\Delta^2(s,n)\cdot\Delta^2(n-1,n)}},\quad s=i,n-3,\quad r_{in-3;n}=\frac{N^3(i,n-3;n)}{\sqrt{\Delta^2(i,n)\cdot\Delta^2(n-3,n)}}.$$

Using these relations and the defining relation (2.3) for the d-scaled partial correlation one obtains

$$\begin{aligned}&N^4(i,n-3;n-1,n)=r_{in-3;n-1n}\cdot\sqrt{\Delta^3(i,n-1,n)\cdot\Delta^3(n-3,n-1,n)}\\&=\left\{\begin{array}{l}\dfrac{N^3(i,n-3;n)\cdot\Delta^2(n-1,n)-N^3(i,n-1;n)\cdot N^3(n-3,n-1;n)}{\Delta^2(n-1,n)\cdot\sqrt{\Delta^2(i,n)\cdot\Delta^2(n-3,n)}}\\ \cdot\dfrac{\sqrt{\Delta^3(i,n-1,n)\cdot\Delta^3(n-3,n-1,n)}}{\sqrt{(1-r_{in-1;n}^2)\cdot((1-r_{n-3n-1;n}^2))}}\end{array}\right\}.\end{aligned}$$

From (2.4) for $n=3$ with index set $s^{(3)}=(s_1,s_2,s_3)=(s,n-1,n)$ one gets $\Delta^3(s,n-1,n)=\Delta^2(s,n)\cdot\Delta^2(n-1,n)\cdot(1-r_{sn-1;n}^2),\quad s=i,n-3$. Inserted into the preceding relation shows the result for $k=4$. It remains to show that if (2.5) holds for the index k then it holds for the index $k+1$. Proceeding similarly one notes that

$$r_{in-k;n-k+2,...,n}=\frac{r_{in-k;n-k+3,...,n}-r_{in-k+2;n-k+3,...,n}\cdot r_{n-kn-k+2;n-k+3,...,n}}{\sqrt{(1-r_{in-k+2;n-k+3,...,n}^2)\cdot((1-r_{n-kn-k+2;n-k+3,...,n}^2))}},$$

with

$$r_{sn-k+2;n-k+3,\ldots,n} = \frac{N^k(s,n-k+2;n-k+3,\ldots,n)}{\sqrt{\Delta^{k-1}(s,n-k+3,\ldots,n)\cdot\Delta^{k-1}(n-k+2,n-k+3,\ldots,n)}}, \quad s=i,n-k,$$

$$r_{in-k;n-k+3,\ldots,n} = \frac{N^k(i,n-k;n-k+3,\ldots,n)}{\sqrt{\Delta^{k-1}(i,n-k+3,\ldots,n)\cdot\Delta^{k-1}(n-k,n-k+3,\ldots,n)}}$$

Inserting these relations into (2.3) one obtains

$$\frac{N^{k+1}(i,n-k;n-k+2,\ldots,n)}{\sqrt{\Delta^k(i,n-k+2,\ldots,n)\cdot\Delta^k(n-k,n-k+2,\ldots,n)}} = r_{in-k;n-k+2,\ldots,n}$$

$$= \frac{\dfrac{N^k(i,n-k;n-k+3,\ldots,n)\cdot\Delta^{k-1}(n-k+2,\ldots,n)}{\Delta^{k-1}(n-k+2,\ldots,n)\cdot\sqrt{\Delta^{k-1}(i,n-k+3,\ldots,n)\cdot\Delta^{k-1}(n-k,n-k+3,\ldots,n)}}}{\sqrt{(1-r^2_{in-k+2;n-k+3,\ldots,n})\cdot(1-r^2_{n-kn-k+2;n-k+3,\ldots,n})}}$$

$$-\frac{\dfrac{N^k(i,n-k+2;n-k+3,\ldots,n)\cdot N^k(n-k,n-k+2;n-k+3,\ldots,n)}{\Delta^{k-1}(n-k+2,\ldots,n)\cdot\sqrt{\Delta^{k-1}(i,n-k+3,\ldots,n)\cdot\Delta^{k-1}(n-k,n-k+3,\ldots,n)}}}{\sqrt{(1-r^2_{in-k+2;n-k+3,\ldots,n})\cdot(1-r^2_{n-kn-k+2;n-k+3,\ldots,n})}}$$

Proposition 2.2 in Hürlimann [4] remains true when replacing the canonical index set by any other index set. In particular (2.8) (loc. cit.) is valid for the index set

$$s^{(k)} = (s_1,\ldots,s_k)\ ,\ s_1 = s\in\{i,n-k\},\ \ s_2 = n-k+2,\ \ s_j = j,\ j=n-k+3,\ldots,n\ ,$$

hence

$$\begin{aligned}&\Delta^k(s,n-k+2,\ldots,n)\cdot\Delta^{k-2}(n-k+3,\ldots,n)\\ &=\Delta^{k-1}(s,n-k+3,\ldots,n)\cdot\Delta^{k-1}(n-k+2,\ldots,n)\cdot(1-r^2_{sn-k+2;n-k+3,\ldots,n}),\quad s=i,n-k.\end{aligned}$$

Inserted into the preceding relation shows (2.5) for the index $k+1$. ◊

3 Cartesian and polar coordinates for the elliptope

As a main result, we derive the following canonical parameterization for correlation matrices. The representation is canonical in the sense that it holds up to a permutation matrix of order n.

Theorem 3.1 (*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

$$r_{in}=x_{in},\quad i=1,\ldots,n-1,\quad n\ge 2, \tag{3.1}$$

$$r_{in-1}=x_{in}x_{n-1n}+x_{in-1}y_{in-1,n},\quad i=1,\ldots,n-2,\quad n\ge 3, \tag{3.2}$$

$$\begin{aligned} r_{in-k} &= x_{in}x_{n-kn}+\sum_{j=2}^{k}x_{in-j+1}x_{n-kn-j+1}\prod_{\ell=n-j+2}^{n}y_{in-k,\ell} \\ &+x_{in-k}\prod_{\ell=n-k+1}^{n}y_{in-k,\ell},\quad i=1,\ldots,n-k-1,\quad k=2,\ldots,n-2,\quad n\ge 4 \end{aligned} \tag{3.3}$$

Corollary 3.1 (*Polar coordinates of* n*-dimensional elliptope*). There exists a bijective mapping between the cube $[-\frac{\pi}{2},\frac{\pi}{2}]^{\frac{1}{2}(n-1)n}$ and E_n, which maps the polar coordinates $\varphi=(\varphi_{ij})$ to $r=(r_{ij})$ such that

$$r_{in}=\sin(\varphi_{in}),\quad i=1,\ldots,n-1,\quad n\ge 2, \tag{3.4}$$

$$r_{in-1}=\left\{\begin{array}{l}\sin(\varphi_{in})\sin(\varphi_{n-1n})\\ +\sin(\varphi_{in-1})\cos(\varphi_{in})\cos(\varphi_{n-1n})\end{array}\right\},\quad i=1,\ldots,n-2,\quad n\ge 3, \tag{3.5}$$

$$r_{in-k}=\left\{\begin{array}{l}\sin(\varphi_{in})\sin(\varphi_{n-kn})\\ +\sum_{j=2}^{k}\sin(\varphi_{in-j+1})\sin(\varphi_{n-kn-j+1})\prod_{\ell=n-j+2}^{n}\cos(\varphi_{i\ell})\cos(\varphi_{n-k\ell})\\ +\sin(\varphi_{in-k})\prod_{\ell=n-k+1}^{n}\cos(\varphi_{i\ell})\cos(\varphi_{n-k\ell})\end{array}\right\}, \tag{3.6}$$

$i=1,\ldots,n-k-1,\quad k=2,\ldots,n-2,\quad n\ge 4.$

Proof Set $x_{ij}=\sin(\varphi_{ij})$ in the formulas of Theorem 3.1. ◊

Remarks 3.1

(i) Researchers in Applied Mathematics often report the difficulty to generate valid correlation (covariance) matrices. For example Hirschberger et al. [2] "were not able to generate a single valid 50x50 covariance matrix by assigning random numbers in 800 tries" and state that "sizes of 1000x1000 are not uncommon" in portfolio selection. Theorem 3.1 solves this practical problem from an algebraic viewpoint. To generate a valid random correlation matrix, it suffices to choose $\frac{1}{2}(n-1)n$ uniform $[-1,1]$ random numbers $x_{ij}, 1 \le i < j \le n$, and apply the formulas (3.1)-(3.3).

(ii) Another different but less general trigonometric approach to correlation matrices than Corollary 3.1 is the hyper-sphere decomposition by Rebonato [6] (see also Brigo [1] and Rebonato [7]).

The derivation of the explicit coordinates (3.1)-(3.3) relies on the following new and more appropriate variant of Theorem 3.1 in Hürlimann [4]. Note the misprint in the denominator of formula (3.4) (loc. cit.), which should be $\Delta^k(n-k+1,...,n)$ as in (3.10) below.

Theorem 3.2 (*Recursive generation of valid correlation matrices*) A correlation matrix parameterized by $r=(r_{ij}), 1 \le i < j \le n$ in E_n, is positive semi-definite if, and only if, the following bounds are fulfilled:

$$r_{in} \in [-1,1] \quad i=1,...,n-1, \quad n \ge 2, \tag{3.7}$$

$$\begin{aligned} &r_{in-1} \in [r_{in-1}^-, r_{in-1}^+], \quad i=1,...,n-2, \quad n \ge 3, \\ &r_{in-1}^{\pm} = r_{in} r_{n-1n} \pm \sqrt{(1-r_{in}^2)(1-r_{n-1n}^2)} \end{aligned} \tag{3.8}$$

$$\begin{aligned} &r_{in-2} \in [r_{in-2}^-, r_{in-2}^+], \quad i=1,...,n-3, \quad n \ge 4, \\ &r_{in-2}^{\pm} = r_{in} r_{n-2n} + \frac{N^3(i,n-1;n) \cdot N^3(n-2,n-1;n)}{1-r_{n-1n}^2} \\ &\pm \frac{\sqrt{\Delta^3(i,n-1,n) \cdot \Delta^3(n-2,n-1,n)}}{1-r_{n-1n}^2} \end{aligned} \tag{3.9}$$

$$\begin{aligned} & r_{in-k} \in [r_{in-k}^-, r_{in-k}^+], \quad i = 1,...,n-k-1, \quad k = 3,...,n-2, \quad n \geq 5, \\ & r_{in-k}^{\pm} = r_{in} r_{n-kn} \\ & + \sum_{j=2}^{k} \frac{N^{j+1}(i, n-j+1; n-j+2,...,n) \cdot N^{j+1}(n-k, n-j+1; n-j+2,...,n)}{\Delta^{j-1}(n-j+2,...,n) \cdot \Delta^{j}(n-j+1,...,n)} \\ & \pm \frac{\sqrt{\Delta^{k+1}(i, n-k+1,...,n) \Delta^{k+1}(n-k, n-k+1,...,n)}}{\Delta^{k}(n-k+1,...,n)} \end{aligned} \tag{3.10}$$

Proof A correlation matrix is positive semi-definite if, and only if, all correlations and partial correlations in the product expansion (2.4) belong to the interval $[-1,1]$ (e.g. Lemma 2.1 in Hürlimann [3]). The bounds are derived in two steps.

Step 1: derivation of (3.7)-(3.9)

From the first product one gets immediately the bounds (3.7). The partial correlations in the second product satisfy the condition

$$r_{in-1;n} = \frac{r_{in-1} - r_{in} r_{n-1n}}{\sqrt{(1-r_{in}^2)(1-r_{n-1n}^2)}} \in [-1,1]$$

if, and only if, one has

$$r_{in-1} \in [r_{in-1}^-, r_{in-1}^+]$$

with $r_{in-1}^{\pm} = r_{in} r_{n-1n} \pm \sqrt{(1-r_{in}^2)(1-r_{n-1n}^2)}$, which shows the bounds (3.8). For the partial correlations in the third product, one sees first that

$$r_{in-2;n-1,n} = \frac{r_{in-2;n} - r_{in-1;n} r_{n-2n-1;n}}{\sqrt{(1-r_{in-1;n}^2)(1-r_{n-2n-1;n}^2)}} \in [-1,1]$$

if, and only if, one has

$$r_{in-2;n} \in [r_{in-2;n}^-, r_{in-2;n}^+]$$

with

$$r_{in-2;n}^{\pm} = r_{in-1;n} r_{n-2n-1;n} \pm \sqrt{(1-r_{in-1;n}^2)(1-r_{n-2n-1;n}^2)} \,.$$

Since

$$r_{in-2;n} = \frac{r_{in-2} - r_{in} r_{n-2n}}{\sqrt{(1-r_{in}^2)(1-r_{n-2n}^2)}}$$

this condition is fulfilled if, and only if, one has

$$r_{in-2} \in [r_{in-2}^-, r_{in-2}^+]$$

with

$$\begin{aligned} r_{in-2}^{\pm} &= r_{in} r_{n-2n} + r_{in-2;n}^{\pm} \sqrt{(1-r_{in}^2)(1-r_{n-2n}^2)} \\ &= r_{in} r_{n-2n} + \{ r_{in-1;n} r_{n-2n-1;n} \pm \sqrt{(1-r_{in-1;n}^2)(1-r_{n-2n-1;n}^2)} \} \sqrt{(1-r_{in}^2)(1-r_{n-2n}^2)}. \end{aligned}$$

But, one has

$$r_{in-1;n} = \frac{r_{in-1} - r_{in} r_{n-1n}}{\sqrt{(1-r_{in}^2)(1-r_{n-1n}^2)}}, \quad r_{n-2n-1;n} = \frac{r_{n-2n-1} - r_{n-2n} r_{n-1n}}{\sqrt{(1-r_{n-2n}^2)(1-r_{n-1n}^2)}},$$

which implies by definition of the d-scaled partial correlations that

$$r_{in-1;n} r_{n-2n-1;n} \sqrt{(1-r_{in}^2)(1-r_{n-2n}^2)} = \frac{N^3(i, n-1; n) \cdot N^3(n-2, n-1; n)}{1 - r_{n-1n}^2}.$$

Furthermore, one has

$$1 - r_{in-1;n}^2 = \frac{\Delta^3(i, n-1, n)}{(1-r_{in}^2)(1-r_{n-1n}^2)}, \quad 1 - r_{n-2n-1;n}^2 = \frac{\Delta^3(n-2, n-1, n)}{(1-r_{n-2n}^2)(1-r_{n-1n}^2)}.$$

By inserting both expressions into the above, one obtains the bounds (3.9).

Step 2: derivation of (3.10)

For each fixed $k = 3, \dots, n-2$ the curly bracket in the last product of (3.11) satisfies the conditions

$$r_{in-k;n-k+1,n} = \frac{r_{in-k;n-k+2,\dots,n} - r_{in-k+1;n-k+2,\dots,n} r_{n-kn-k+1;,n-k+2,\dots,n}}{\sqrt{(1-r_{in-k+1;n-k+2,\dots,n}^2)(1-r_{n-kn-k+1;n-k+2,\dots,n}^2)}} \in [-1,1], \quad i = 1, \dots, n-k-1,$$

if, and only if, one has $r_{in-k;n-k+2,\dots,n} \in [r_{in-k;n-k+2,\dots,n}^-, r_{in-k;n-k+2,\dots,n}^+]$ with

$$\begin{aligned} r_{in-k;n-k+2,\dots,n}^{\pm} &= r_{in-k+1;n-k+2,\dots,n} r_{n-kn-k+1;n-k+2,\dots,n} \\ &\pm \sqrt{(1-r_{in-k+1;n-k+2,\dots,n}^2)(1-r_{n-kn-k+1;n-k+2,\dots,n}^2)}. \end{aligned}$$

Since

$$r_{in-k;n-k+2,...,n} = \frac{r_{in-k;n-k+3,...,n} - r_{in-k+2;n-k+3,...,n} r_{n-kn-k+2;n-k+3,...,n}}{\sqrt{(1-r^2_{in-k+2;n-k+3,...,n})(1-r^2_{n-kn-k+2;n-k+3,...,n})}}$$

this condition is fulfilled if, and only if, one has

$$r_{in-k;n-k+3,...,n} \in [r^-_{in-k;n-k+3,...,n}, r^+_{in-k;n-k+3,...,n}]$$

with

$$\begin{aligned}
&r^{\pm}_{in-k;n-k+3,...,n} = r_{in-k+2;n-k+3,...,n} r_{n-kn-k+2;n-k+3,...,n} \\
&+ r^{\pm}_{in-k;n-k+2,...,n} \sqrt{(1-r^2_{in-k+2;n-k+3,...,n})(1-r^2_{n-kn-k+2;n-k+3,...,n})} \\
&= r_{in} r_{n-2n} + \{ r_{in-k+1;n-k+2,...,n} r_{n-kn-k+1;n-k+2,...,n} \\
&\pm \sqrt{(1-r^2_{in-k+1;n-k+2,...,n})(1-r^2_{n-kn-k+1;n-k+2,...,n})} \} \sqrt{(1-r^2_{in})(1-r^2_{n-2n})}.
\end{aligned}$$

One continues this way until $r_{in-k} \in [r^-_{in-k}, r^+_{in-k}]$ with (proof by induction on k)

$$\begin{aligned}
r^{\pm}_{in-k} = r_{in} \cdot r_{n-kn} + \sum_{j=2}^{k} &\left\{ \begin{array}{l} r_{in-j+1;n-j+2,...,n} \cdot r_{n-kn-j+1;n-j+2,...,n} \cdot \sqrt{(1-r^2_{in}) \cdot (1-r^2_{n-kn})} \\ \cdot \prod_{s=2}^{j-1} \sqrt{(1-r^2_{in-s+1;n-s+2,...,n}) \cdot (1-r^2_{n-kn-s+1;n-s+2,...,n})} \end{array} \right\} \qquad (3.11) \\
\pm \sqrt{(1-r^2_{in}) \cdot (1-r^2_{n-kn})} \cdot &\prod_{s=2}^{k} \sqrt{(1-r^2_{in-s+1;n-s+2,...,n}) \cdot (1-r^2_{n-kn-s+1;n-s+2,...,n})}
\end{aligned}$$

One must show that (3.11) coincides with (3.10). For $j = 2$ one has by Definition (2.3)

$$r_{in-1;n} = \frac{N^3(i, n-1; n)}{\sqrt{(1-r^2_{in})(1-r^2_{n-1n})}}, \quad i = 1,...,n-k, \text{ hence}$$

$$r_{in-1;n} r_{n-kn-1;n} \sqrt{(1-r^2_{in})(1-r^2_{n-kn})} = \frac{N^3(i, n-1; n) \cdot N^3(n-k, n-1; n)}{1-r^2_{n-1n}},$$

which coincides with the term for $j = 2$ in the second sum of (3.10). Similarly, for $j = 3,...,k$ one has by Definition (2.3)

$$r_{in-j+1;n-j+2,...,n} = \frac{N^{j+1}(i, n-j+1; n-j+2,...,n)}{\sqrt{\Delta^j(i, n-j+2, n) \cdot \Delta^j(n-j+1, n-j+2,...,n)}}, \qquad (3.12)$$
$$i = 1,...,n-k.$$

On the other hand, from a general version of (2.4) with arbitrary index set, one obtains for $j=3,...,k+1$ the recursive relationships

$$\Delta^{j}(i,n-j+2,...,n)=\Delta^{j-1}(n-j+2,...,n)\cdot(1-r_{in}^{2})\cdot\prod_{s=2}^{j-1}(1-r_{in-s+1;n-s+2,...,n}^{2}),\quad i=1,...,n-j+1. \tag{3.13}$$

If one combines (3.12) and (3.13), one sees that the terms for $j=3,...,k$ in the second sum of (3.11) coincide with the corresponding terms in (3.10). Finally, using (3.13) for $j=k+1$ shows that the last term in (3.11) coincides with the last term in (3.10). The result is shown. ◊

Before entering into the proof of Theorem 3.1, it is necessary to explain how the coordinates $x_{ij}\in[-1,1]$ are actually defined. Clearly, the formulas (3.1)-(3.2) are restatements of the bounds (3.7)-(3.8) and show how $x_{in},x_{in-1}\in[-1,1]$ are chosen. Similarly, to satisfy the bounds (3.9)-(3.10) it suffices to define r_{in-k} through these formulas by multiplying the square root terms with $x_{in-k}\in[-1,1]$, where $i=1,...,n-3$ when $k=2,\ n\geq 4$, and $i=1,...,n-k-1$ when $k=3,...n-2,\ n\geq k+2$. This settles uniquely the choice of $x=(x_{ij})\in[-1,1]^{\frac{1}{2}(n-1)n}$. Now, the derivation of the Cartesian coordinates depends upon the following main auxiliary identity, whose proof is postponed to Section 4.

Lemma 3.1 For all $i=1,...,n-k,\quad k=2,...,n-2,\quad n\geq 4,$ one has the identity

$$N^{k+1}(i,n-k+1;n-k+2,...,n)=x_{in-k+1}\cdot\sqrt{\Delta^{k}(i,n-k+2,...,n)\cdot\Delta^{k}(n-k+1,...,n)}\,.$$

Corollary 3.1 For all $i=1,...,n-k,\quad k=2,...,n-2,\quad n\geq 4,$ one has the identity

$$\Delta^{k+1}(i,n-k+1,...,n)=\Delta^{k}(n-k+1,...,n)\cdot\prod_{\ell=n-k+1}^{n}(1-x_{i\ell}^{2})\,.$$

Proof This is shown by induction. For $k=2,\ n\geq 4$, one has

$$\Delta^3(i,n-1,n)=1-r_{in-1}^2-x_{in}^2-x_{n-1n}^2+2r_{in-1}x_{in}x_{n-1n}.$$

Since (3.2) is just a restatement of the bounds (3.8), one has $r_{in-1}=x_{in}x_{n-1n}+x_{in-1}y_{in-1,n}$, hence

$$\begin{aligned}&\Delta^3(i,n-1,n)=1-x_{in}^2x_{n-1n}^2-2x_{in}x_{n-1n}x_{in-1}y_{in-1,n}-x_{in-1}^2(1-x_{in}^2)(1-x_{n-1n}^2)\\&-x_{in}^2-x_{n-1n}^2+2x_{in}^2x_{n-1n}^2+2x_{in}x_{n-1n}x_{in-1}y_{in-1,n}\\&=(1-x_{in}^2)-x_{in}^2(1-x_{n-1n}^2)-x_{in-1}^2(1-x_{in}^2)(1-x_{n-1n}^2)\\&=(1-x_{n-1n}^2)\cdot\prod_{\ell=n-1}^{n}(1-x_{i\ell}^2)=\Delta^2(n-1,n)\cdot\prod_{\ell=n-1}^{n}(1-x_{i\ell}^2),\end{aligned}$$

as should be. Now, assume the identity holds for the index $k-1$ and show it for the index k. From Proposition 2.2 in Hürlimann [4] one borrows the identity

$$\begin{aligned}&\Delta^{k+1}(i,n-k+1,...,n)\cdot\Delta^{k-1}(n-k+2,...,n)\\&=\Delta^k(i,n-k+2,...,n)\cdot\Delta^k(n-k+1,...,n)-N^{k+1}(i,n-k+1;n-k+2,...,n)^2.\end{aligned}$$

With the Lemma 3.1 this can be rewritten as

$$\Delta^k(n-k+1,...,n)\cdot(1-x_{in-k+1}^2)\cdot\Delta^k(i,n-k+2,...,n),$$

which by induction assumption is equal to

$$\Delta^k(n-k+1,...,n)\cdot(1-x_{in-k+1}^2)\cdot\Delta^{k-1}(n-k+2,...,n)\cdot\prod_{\ell=n-k+2}^{n}(1-x_{i\ell}^2).$$

Dividing both sides of the identity by $\Delta^{k-1}(n-k+2,...,n)$ shows the desired identity for the index k. Corollary 3.1 is shown. ◊

Proof of Theorem 3.1 As already made clear, the formulas (3.1)-(3.2) are restatements of the bounds (3.7)-(3.8). In a first step, one shows the validity of (3.3) for $k=2,\ i=1,...,n-3,\ n\geq 4$. From the bounds (3.9) one has for some $x_{in-2}\in[-1,1]$ the identity

$$r_{in-2} = r_{in} r_{n-2n} + \frac{N^3(i,n-1;n)\cdot N^3(n-2,n-1;n)}{1-r_{n-1n}^2} + x_{in-2}\,\frac{\sqrt{\Delta^3(i,n-1,n)\cdot\Delta^3(n-2,n-1,n)}}{1-r_{n-1n}^2}.$$

Clearly, the first term coincides with $x_{in}x_{n-2n}$. For the middle term, use Lemma 3.1 to see that

$$N^3(i,n-1;n) = x_{in-1}\cdot\sqrt{(1-x_{in}^2)(1-x_{n-1n}^2)},$$

$$N^3(n-2,n-1;n) = x_{n-2n-1}\cdot\sqrt{(1-x_{n-2n}^2)(1-x_{n-1n}^2)},$$

which implies that

$$\frac{N^3(i,n-1;n)\cdot N^3(n-2,n-1;n)}{1-r_{n-1n}^2} = x_{in-1}x_{n-2n-1}y_{in-2,n}.$$

On the other hand, Corollary 3.1 shows that

$$\Delta^3(i,n-1,n) = (1-x_{n-1n}^2)\prod_{\ell=n-1}^{n}(1-x_{i\ell}^2),$$

$$\Delta^3(n-2,n-1,n) = (1-x_{n-1n}^2)\prod_{\ell=n-1}^{n}(1-x_{n-2\ell}^2).$$

Inserted into the third term yields

$$\frac{\sqrt{\Delta^3(i,n-1,n)\cdot\Delta^3(n-2,n-1,n)}}{1-r_{n-1n}^2} = \prod_{\ell=n-1}^{n}\sqrt{(1-x_{i\ell}^2)(1-x_{n-2\ell}^2)} = \prod_{\ell=n-1}^{n} y_{in-2,\ell}.$$

Together, this shows (3.3) for $k=2,\, n\ge 4$. Now, let $i=1,...,n-k-1,\ k=3,...,n-2,\ n\ge 5$. From the bounds (3.10) one has for some $x_{in-k}\in[-1,1]$ the identity

$$\begin{aligned} r_{in-k} &= r_{in}r_{n-kn} \\ &+ \sum_{j=2}^{k}\frac{N^{j+1}(i,n-j+1;n-j+2,...,n)\cdot N^{j+1}(n-k,n-j+1;n-j+2,...,n)}{\Delta^{j-1}(n-j+2,...,n)\cdot\Delta^{j}(n-j+1,...,n)} \\ &+ x_{in-k}\,\frac{\sqrt{\Delta^{k+1}(i,n-k+1,...,n)\Delta^{k+1}(n-k,n-k+1,...,n)}}{\Delta^{k}(n-k+1,...,n)}. \end{aligned}$$

One argues similarly to the above. The first term coincides with $x_{in}x_{n-kn}$. For the summands of the middle term one has with Lemma 3.1 that

$$N^{j+1}(i,n-j+1;n-j+2,...,n)$$
$$=x_{in-j+1}\cdot\sqrt{\Delta^{j}(i,n-j+2,...,n)\cdot\Delta^{j}(n-j+1,...,n)},$$
$$N^{j+1}(n-k,n-j+1;n-j+2,...,n)$$
$$=x_{n-kn-j+1}\cdot\sqrt{\Delta^{j}(n-k,n-j+2,...,n)\cdot\Delta^{j}(n-j+1,...,n)},$$

which implies that

$$\frac{N^{j+1}(i,n-j+1;n-j+2,...,n)\cdot N^{j+1}(n-k,n-j+1;n-j+2,...,n)}{\Delta^{j-1}(n-j+2,...,n)\cdot\Delta^{j}(n-j+1,...,n)}$$
$$=x_{in-j+1}x_{n-kn-j+1}\frac{\sqrt{\Delta^{j}(i,n-j+2,...,n)\Delta^{j}(n-k,n-j+1,...,n)}}{\Delta^{j-1}(n-j+2,...,n)}.$$

Through application of Corollary 3.1 one obtains further

$$\Delta^{j}(i,n-j+2,...,n)=\Delta^{j-1}(n-j+2,...,n)\cdot\prod_{\ell=n-j+2}^{n}(1-x_{i\ell}^{2}),$$
$$\Delta^{j}(n-k,n-j+2,...,n)=\Delta^{j-1}(n-j+2,...,n)\cdot\prod_{\ell=n-j+2}^{n}(1-x_{n-k\ell}^{2}).$$

Therefore, the preceding term coincides with

$$x_{in-j+1}x_{n-kn-j+1}\cdot\prod_{\ell=n-j+2}^{n}\sqrt{(1-x_{i\ell}^{2})(1-x_{n-k\ell}^{2})}=x_{in-j+1}x_{n-kn-j+1}\cdot\prod_{\ell=n-j+2}^{n}y_{in-k,\ell}\,.$$

Finally, for the last term, one obtains from Corollary 3.1 that

$$x_{in-k}\frac{\sqrt{\Delta^{k+1}(i,n-k+1,...,n)\Delta^{k+1}(n-k,n-k+1,...,n)}}{\Delta^{k}(n-k+1,...,n)}$$
$$=x_{in-k}\prod_{\ell=n-k+1}^{n}\sqrt{(1-x_{i\ell}^{2})(1-x_{n-k\ell}^{2})}=x_{in-k}\prod_{\ell=n-k+1}^{n}y_{in-k,\ell}.$$

Together, this shows (3.3) for $k=3,...,n-2,\ n\geq 5$. The proof is complete. ◊

4 Derivation of the remaining main auxiliary identity

It remains to show the validity of Lemma 3.1. We show the following slightly more general identity, which for $s=-1$ reduces to Lemma 3.1.

Lemma 4.1 For all $i=1,...,n-k$, $k=2,...,n-2$, $s=-1,0,1,...,k-3$, $n\ge 4$, one has the identity

$$N^{k-s}(i,n-k+1;n-k+s+3,...,n)=\Delta^{k-s-2}(n-k+s+3,...,n) \\ \cdot\left(\sum_{j=0}^{s} x_{in-k+j+2}x_{n-k+1n-k+j+2}\prod_{\ell=n-k+j+3}^{n} y_{in-k+1,\ell}+x_{in-k+1}\prod_{\ell=n-k+2}^{n} y_{in-k+1,\ell}\right) \tag{4.1}$$

Proof This is shown by forward induction on the index k (with arbitrary s) and backward induction on the index s (with arbitrary k). If $k=2$ one has necessarily $s=-1$. Then from (3.2) of Theorem 3.1 (that is trivially true as already mentioned) one gets

$$N^{3}(i,n-1;n)=r_{in-1}-r_{in}r_{n-1n}=x_{in-1}\cdot\sqrt{(1-x_{in}^{2})(1-x_{n-1n}^{2})}\,.$$

Now, assume that (4.1) is true for all indices less than or equal to $k-1$ and show it for the index k. In particular, Lemma 3.1 is true for the index $k-1$ and in virtue of the proof of Theorem 3.1, the identity (3.3) is also true for the index $k-1$, a property which is used to settle the base case $s=k-3$. Indeed, for this index the identity (4.1) follows from (3.3) with index $k-1$ because

$$\begin{aligned} &N^{3}(i,n-k+1;n)=r_{in-(k-1)}-r_{in}r_{n-k+1n} \\ &=\sum_{j=2}^{k-1} x_{in-j+1}x_{n-k+1n-j+1}\prod_{\ell=n-j+2}^{n} y_{in-k+1,\ell}+x_{in-k+1}\prod_{\ell=n-k+2}^{n} y_{in-k+1,\ell} \\ &=\sum_{j=0}^{k-3} x_{in-k+j+2}x_{n-k+1n-k+j+2}\prod_{\ell=n-k+j+3}^{n} y_{in-k+1,\ell}+x_{in-k+1}\prod_{\ell=n-k+2}^{n} y_{in-k+1,\ell}\,. \end{aligned}$$

Now, by Proposition 2.1 one has the identity

$$\begin{aligned} &N^{k-s}(i,n-k+1;n-k+s+3,...,n)\cdot\Delta^{k-s-3}(n-k+s+4,...,n) \\ &=N^{k-s-1}(i,n-k+1;n-k+s+4,...,n)\cdot\Delta^{k-s-2}(n-k+s+3,...,n) \\ &-\left\{\begin{array}{l} N^{k-s-1}(i,n-k+s+3;n-k+s+4,...,n) \\ \cdot N^{k-s-1}(n-k+1,n-k+s+3;n-k+s+4,...,n) \end{array}\right\}. \end{aligned}$$

By the backward induction assumption with index $s+1$ the identity (4.1) yields

$$N^{k-s-1}(i,n-k+1;n-k+s+4,...,n)=\Delta^{k-s-3}(n-k+s+4,...,n)$$
$$\cdot(\sum_{j=0}^{s+1}x_{in-k+j+2}x_{n-k+1n-k+j+2}\prod_{\ell=n-k+j+3}^{n}y_{in-k+1,\ell}+x_{in-k+1}\prod_{\ell=n-k+2}^{n}y_{in-k+1,\ell}).$$

By the forward induction assumption the identity of Lemma 3.1 yields

$$N^{k-s-1}(i,n-k+s+3;n-k+s+4,...,n)$$
$$=x_{in-k+s+3}\cdot\sqrt{\Delta^{k-s-2}(i,n-k+s+4,...,n)\cdot\Delta^{k-s-2}(n-k+1,n-k+s+4,...,n)},$$
$$N^{k-s-1}(i,n-k+s+3;n-k+s+4,...,n)$$
$$=x_{in-k+s+3}\cdot\sqrt{\Delta^{k-s-2}(i,n-k+s+4,...,n)\cdot\Delta^{k-s-2}(n-k+1,n-k+s+4,...,n)}.$$

Inserted into the above one gets

$$N^{k-s}(i,n-k+1;n-k+s+3,...,n)\cdot\Delta^{k-s-3}(n-k+s+4,...,n)$$
$$=\Delta^{k-s-2}(n-k+s+3,...,n)\cdot\Delta^{k-s-3}(n-k+s+4,...,n)$$
$$\cdot(\sum_{j=0}^{s}x_{in-k+j+2}x_{n-k+1n-k+j+2}\prod_{\ell=n-k+j+3}^{n}y_{in-k+1,\ell}+x_{in-k+1}\prod_{\ell=n-k+2}^{n}y_{in-k+1,\ell}).$$

Divide by $\Delta^{k-s-3}(n-k+s+4,...,n)$ to obtain the desired expression (4.1). ◊

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