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Direct formulation to Cholesky decomposition of a general nonsingular correlation matrix[☆]

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ABSTRACT

We present two novel and explicit parametrizations of Cholesky factor of a nonsingular correlation matrix. One that uses semi-partial correlation coefficients, and a second that utilizes differences between the successive ratios of two determinants. To each, we offer a useful application.

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1. Cholesky decomposition—Introduction

For a positive-definite symmetric matrix Cholesky decomposition provides a unique representation in the form of $\mathbf{LL}^T$, with a lower triangular matrix $\mathbf{L}$ and the upper triangular $\mathbf{L}^T$. Offered by a convenient $O(n^3)$ algorithm, Cholesky decomposition is favored by many for expressing the covariance matrix (Pourahmadi, 2011). The matrix $\mathbf{L}$ itself can be used to transform independent normal variables into dependent multinormal (Moonan, 1957) which is particularly useful for Monte Carlo simulations.

Explicit forms of $\mathbf{L}$ are known for limited correlation structures such as the equicorrelated (Tong, 1990, p. 104), tridiagonal (Miwa et al., 2003), and the multinomial (Tanabe and Sagae, 1992). The general correlated case is typically computed by using spherical parametrizations (Pinheiro and Bates, 1996; Rapisarda et al., 2007; Rebonato and Jackel, 2000; Mittelbach et al., 2012), a multiplicative ensemble of trigonometric functions of the angles between pairs of vectors. Others may use Cholesky matrix (Cooke et al., 2011, p. 49) that utilizes the multiplication of partial correlations.

In this paper, we will present two explicit parametrizations of Cholesky factor for a positive-definite correlation matrix. Both parametrizations offer a preferable, simpler alternatives to the multiplicative forms of spherical parametrization and partial correlations. In Section 2 we show that the nonzero elements of Cholesky factor are the *semi-partial correlation coefficients*

$$\rho_{ij(1,\ldots,i-1)} = \frac{\rho_{ij} - \boldsymbol{\rho}_i^{*j}\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i}{\sqrt{1 - \boldsymbol{\rho}_i\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T}},$$

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where $\mathbf{R}_{i-1}^{-1}$ is the inverse of the correlation matrix $\mathbf{R}_i = (\rho_{kj})_{k,j=1}^{i-1}$, $\boldsymbol{\rho}_i^{*j} = (\rho_{1j}, \rho_{2j}, \ldots, \rho_{i-1,j})$ and $\boldsymbol{\rho}_i = \boldsymbol{\rho}_i^{*i}$. The order of the $\boldsymbol{\rho}_{ij(1,\ldots,i-1)}$s is determined by Cholesky factorization, and the notations are borrowed from Huber's trivariate discussion of semi-partial correlation in regression (Huber, 1981). In Section 3 we uncover that the squares, $\boldsymbol{\rho}^2_{ij(1,\ldots,i-1)}$, are equivalent to the differences between two successive ratios of determinants, and we use this equivalence to construct the second parametrization for $\mathbf{L}$. In Section 3.1 we extend the representation of $\mathbf{L}$ to the structure of a covariance matrix, and in Section 3.2 we study two inequality conditions that are essential for the positive-definiteness of $\mathbf{LL}^T$. We conclude this paper by offering two possible applications, one for each of the suggested forms. In Section 4 we present a simple t-test that employs the semi-partial correlation structure for testing the dependence of a single variable upon a set of multivariate normals. In Section 5 we utilize the second parametrization to design a simple algorithm for the generation of random positive-definite correlation matrices. We end the paper with the simple case of generalization of random AR(1) correlation in Section 5.1.

2. The first parametrization for Cholesky factor

Let $\mathbf{R}_n = (\rho_{ij})_{ij=1}^n$ be a positive-definite correlation matrix, for which each sub-matrix $\mathbf{R}_k = (\rho_{ij})_{ij=1}^k$ is positive-definite. Let also $\mathbf{L} = (l_{ij})_{ij=1}^n$ be Cholesky factor of $\mathbf{R}$, $|\mathbf{R}|$ be the determinant of $\mathbf{R}$, $\mathbf{R}^{-1}$ its inverse, and $\boldsymbol{\rho}_i^{*j} = (\rho_{1j}, \rho_{2j}, \ldots, \rho_{i-1,j})$ for $j \geq i$, so $\boldsymbol{\rho}_i \equiv \boldsymbol{\rho}_i^{*i}$. To simplify writing also set $\mathbf{R}_0^{-1} \equiv 1$. The first representation of $\mathbf{L}$ will use the semi-partial correlations $l_{ji} = \boldsymbol{\rho}_{ij(1,\ldots,i-1)} = \frac{\rho_{ij} - \boldsymbol{\rho}_i^{*j}\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T}{\sqrt{1-\boldsymbol{\rho}_i\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T}}, i \leq j,$

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \rho_{12} & \sqrt{1-\rho_{12}^2} & 0 & \cdots & 0 \\ \rho_{13} & \dfrac{\rho_{23} - \rho_{12}\rho_{13}}{\sqrt{1-\rho_{12}^2}} & \sqrt{1-\boldsymbol{\rho}_3\mathbf{R}_2^{-1}\boldsymbol{\rho}_3^T} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ \rho_{1n} & \dfrac{\rho_{2n} - \rho_{12}\rho_{1n}}{\sqrt{1-\rho_{12}^2}} & \dfrac{\rho_{3n} - \boldsymbol{\rho}_3^{*n}\mathbf{R}_2^{-1}\boldsymbol{\rho}_3^T}{\sqrt{1-\boldsymbol{\rho}_3\mathbf{R}_2^{-1}\boldsymbol{\rho}_3^T}} & \cdots & \sqrt{1-\boldsymbol{\rho}_n\mathbf{R}_{n-1}^{-1}\boldsymbol{\rho}_n^T} \end{pmatrix}. \quad (1)$$

For $i = j$, we have $\rho_{ii(1,\ldots,i-1)} = \sqrt{1-\boldsymbol{\rho}_i\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T}$, and $1 - \boldsymbol{\rho}_i\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T > 0$ for positive-definite $\mathbf{R}_i$. Some may recognize the quantity $1 - \boldsymbol{\rho}_i\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T$ as the *schur-complement* of the matrix $\mathbf{R}_{i-1}$ inside $\mathbf{R}_i$ from the formula for computing the determinant of $\mathbf{R}_i$, using the block matrix $\mathbf{R}_{i-1}$ (Harville, 1997, p. 188),

$$|\mathbf{R}_i| = \begin{vmatrix} \mathbf{R}_{i-1} & \boldsymbol{\rho}_i^T \\ \boldsymbol{\rho}_i & 1 \end{vmatrix} = |\mathbf{R}_{i-1}|(1 - \boldsymbol{\rho}_i\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T). \quad (2)$$

To show that $\mathbf{R}_n = \mathbf{LL}^T$ we introduce Theorem 1.

Theorem 1. *For $i \geq 1$ and $n \geq j \geq i+1$,*

$$\boldsymbol{\rho}_{i+1}^{*j}\mathbf{R}_i^{-1}\boldsymbol{\rho}_{i+1}^T = \sum_{k=1}^{i} \rho_{k,i+1(1,\ldots,k-1)} \cdot \rho_{kj(1,\ldots,k-1)}. \quad (3)$$

By the virtue that Cholesky factor of a positive-definite matrix has a unique representation, Theorem 1 will serve as a general proof for the form (1). Some may recognize Eq. (3) in Theorem 1 as the inner-product used for the familiar algorithm of Cholesky Decomposition (Harville, 1997, p. 235):

$$l_{ii} = \left(1 - \sum_{k=1}^{i-1} l_{ik}^2\right)^{1/2} \quad \text{and} \quad l_{ji} = \left(\rho_{ij} - \sum_{k=1}^{i-1} l_{jk}l_{ik}\right) \Big/ l_{ii}.$$

Surprisingly, the equality in Theorem 1 seems to be unknown or neglected. The proof for Theorem 1 will be given in Appendix A, and will be heavily based on the recursive arguments of Lemma 2:

Lemma 2. *For $i \geq 1$ and $n \geq j \geq i+1$,*

$$\boldsymbol{\rho}_{i+1}^{*j}\mathbf{R}_i^{-1}\boldsymbol{\rho}_{i+1}^T = \boldsymbol{\rho}_i^{*j}\mathbf{R}_{i-1}^{-1}(\boldsymbol{\rho}_i^{*i+1})^T + \frac{(\rho_{i,i+1} - \boldsymbol{\rho}_i^{*i+1}\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T)(\rho_{ij} - \boldsymbol{\rho}_i^{*j}\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T)}{1 - \boldsymbol{\rho}_i\mathbf{R}_{i-1}^{-1}\boldsymbol{\rho}_i^T}. \quad (4)$$

The proof for Lemma 2 will be given in Appendix B.