МАТЕМАТИКА И МАТЕМАТИЧЕСКО ОБРАЗОВАНИЕ, 2006
MATHEMATICS AND EDUCATION IN MATHEMATICS, 2006
Proceedings of the Thirty Fifth Spring Conference of
the Union of Bulgarian Mathematicians
Borovets, April 5–8, 2006

UNIFORM RANDOM POSITIVE DEFINITE MATRIX GENERATION*

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In this paper we consider statistics, which have joint uniform distribution on the set of all positively definite matrices with preliminary fixed diagonal elements. We give an algorithm for generation of random uniformly distributed positively definite matrices.

A sufficient condition for applying many numerical algorithms is the positive definiteness of a matrix. The diagonal elements of the matrix have often specified significance. The correctness of such numerical algorithm can be proven if we are able to choose a positively definite matrix uniformly at random. The space of all positively definite matrices is, however, a cone (see [3]) and consequently a uniform distribution cannot be defined over the whole cone because it has infinite volume. This enforces to introduce additional restrictions on the matrices, which together with the positive definiteness reduce our choice within a set with finite volume. This paper suggests an algorithm for generation of uniform distributed positively definite matrices with fixed diagonal elements. If the user does not want to fix concrete diagonal elements of the matrix in advance, he has though to assign bounds for each diagonal element. For instance, he can choose all diagonal elements to be in the interval (0,100). Then uniform random numbers within the chosen bounds have to be generated one for each diagonal element. The algorithm described in this paper allows the user a random choice among all positively definite matrices with concrete diagonal elements that are either fixed in advance or randomly generated within the chosen bounds.

From now on we will assume that $a_{11}, \ \ldots, a_{nn}$ are the diagonal elements of the matrix, chosen in accordance with users' preferences. They have to be positive so that there exists at least one positively definite matrix with such diagonal elements (see Lemma 1 below).

Let us denote by $\Psi(k)$, $k > -1$ the Pearson probability distribution of the second type with density function

$$f_k = \frac{\Gamma\left(\dfrac{k+2}{2}\right)}{\Gamma\left(\dfrac{k+1}{2}\right)\Gamma\left(\dfrac{1}{2}\right)}(1-y^2)^{\frac{k-1}{2}}, \quad y \in (-1,1).$$

***2000 Mathematics Subject Classification:** 62H10

Random variables having distribution $\Psi(k)$ can be easily generated (see [1], p.481) using the quotient of the difference and the sum of two gamma distributed random variables.

Theorem 1. *Let the random variables η_{ij}, $1 \le i < j \le n$ be mutually independent. Suppose that $\eta_{i\,i+1}, \ldots, \eta_{in}$ are identically distributed $\Psi(n-i)$, for $i = 1, \ldots, n-1$. Consider the random variables ν_{ij}, $1 \le i < j \le n$, defined by*

$$\nu_{12} = \eta_{12}\sqrt{a_{11}a_{22}}, \ldots, \nu_{1n} = \eta_{1n}\sqrt{a_{11}a_{nn}};$$

(1)

$$\nu_{ij} = \frac{-\begin{vmatrix} a_{11} & \cdots & \nu_{1\,i-1} & \nu_{1i} \\ \vdots & \ddots & \vdots & \vdots \\ \nu_{1\,i-1} & \cdots & a_{i-1i-1} & \nu_{i-1\,i} \\ \nu_{1j} & \cdots & \nu_{i-1\,j} & 0 \end{vmatrix} + \eta_{ij} \begin{vmatrix} a_{11} & \cdots & \nu_{1\,i} \\ \vdots & \ddots & \vdots \\ \nu_{1\,i} & \cdots & a_{ii} \end{vmatrix}^{1/2} \begin{vmatrix} a_{11} & \cdots & \nu_{1\,i-1} & \nu_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ \nu_{1\,i-1} & \cdots & a_{i-1i-1} & \nu_{i-1\,j} \\ \nu_{1j} & \cdots & \nu_{i-1\,j} & a_{j\,j} \end{vmatrix}^{1/2}}{\begin{vmatrix} a_{11} & \cdots & \nu_{1\,i-1} \\ \vdots & \ddots & \vdots \\ \nu_{1\,i-1} & \cdots & a_{i-1i-1} \end{vmatrix}},$$

$i = 2, \ldots, n-1$, $j = i+1, \ldots, n$.

The joint density of the random variables ν_{ij}, $1 \le i < j \le n$ has the form

$$g_{\nu_{ij},\,1\le i<j\le n}(x_{ij},\, 1 \le i < j \le n) = C I_S,$$

where C is a constant and I_S is the indicator of the set S, consisting of all points $(x_{ij}$, $1 \le i < j \le n)$ in $R_{n(n-1)/2}$, for which the matrix

(2)
$$\mathbf{A} = \begin{pmatrix} a_{11} & x_{12} & \cdots & x_{1n} \\ x_{12} & a_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1n} & x_{2n} & \cdots & a_{nn} \end{pmatrix}$$

is positively definite.

Proof. It is easy to get the joint density of the random variables η_{ij}, $1 \le i < j \le n$:

$$f_{\eta_{ij},1\le i<j\le n}(y_{ij}, 1\le i<j\le n) = f_{n-1}(y_{12})\ldots f_{n-1}(y_{1n}) f_{n-2}(y_{23})\ldots f_{n-2}(y_{2n})\ldots f_1(y_{n-1n}) I_{S'}$$
$$= K_n \prod_{1\le i<j\le n} (1-y_{ij}^2)^{\frac{n-i-1}{2}} I_{S'},$$

where I'_S is the indicator of the set of all points $(y_{ij},\, 1 \le i < j \le n)$ in $R_{n(n-1)/2}$ such that $y_{ij} \in (-1,1)$, $1 \le i < j \le n$ and K_n is the constant

$$K_n = \frac{\left[\Gamma\left(\frac{n+1}{2}\right)\right]^{n-1}}{\Gamma\left(\frac{n}{2}\right)\Gamma\left(\frac{n-1}{2}\right)\ldots\Gamma\left(\frac{3}{2}\right)\left[\Gamma\left(\frac{1}{2}\right)\right]^{\frac{n\,(n-1)}{2}}}.$$

The inverse transformation formulas are of the form

$$y_{12} = x_{12}/\sqrt{a_{11}a_{22}}, \quad \ldots, \quad y_{1n} = x_{1n}/\sqrt{a_{11}a_{nn}};$$

$$
(3) \qquad y_{ij} = \frac{\begin{vmatrix} a_{11} & \cdots x_{1\,i-1} & x_{1i} \\ \vdots & \ddots \vdots & \vdots \\ x_{1\,i-1} & \cdots a_{i-1i-1} & x_{i-1\,i} \\ x_{1j} & \cdots x_{i-1\,j} & 0 \end{vmatrix} + x_{ij} \begin{vmatrix} a_{11} & \cdots x_{1\,i-1} \\ \vdots & \ddots \vdots \\ x_{1\,i-1} & \cdots a_{i-1i-1} \end{vmatrix}}{\begin{vmatrix} a_{11} & \cdots x_{1\,i} \\ \vdots & \ddots \vdots \\ x_{1\,i} & \cdots a_{i\,i} \end{vmatrix}^{1/2} \begin{vmatrix} a_{11} & \cdots x_{1\,i-1} & x_{1j} \\ \vdots & \ddots \vdots & \vdots \\ x_{1\,i-1} & \cdots a_{i-1i-1} & x_{i-1\,j} \\ x_{1j} & \cdots x_{i-1\,j} & a_{j\,j} \end{vmatrix}^{1/2}},
$$

$i = 2, \ldots, n-1$, $j = i+1, \ldots, n$.

It is easy to see that all elements above the main diagonal in the Jacobian $\mathbf{J}$,

$$
\mathbf{J} = \frac{\partial \left(y_{12}, \ldots, y_{1n}, y_{23}, \ldots, y_{2n}, \ldots, y_{n-1n}\right)}{\partial \left(x_{12}, \ldots, x_{1n}, x_{23}, \ldots, x_{2n}, \ldots, x_{n-1n}\right)}
$$

are equal to zero. Consequently,

$$
|\mathbf{J}| = \frac{\partial\, y_{12}}{\partial\, x_{12}} \cdots \frac{\partial\, y_{1n}}{\partial\, x_{1n}} \frac{\partial\, y_{23}}{\partial\, x_{23}} \cdots \frac{\partial\, y_{2n}}{\partial\, x_{2n}} \cdots \frac{\partial\, y_{n-1n}}{\partial\, x_{n-1n}} = \frac{1}{\sqrt{a_{11}a_{22}}} \cdots \frac{1}{\sqrt{a_{11}a_{nn}}}
$$

$$
\times \prod_{2 \le i < j \le n} \frac{\begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} \\ \vdots & \ddots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} \end{vmatrix}}{\begin{vmatrix} a_{11} & \cdots & x_{1\,i} \\ \vdots & \ddots & \vdots \\ x_{1\,i} & \cdots & a_{ii} \end{vmatrix}^{1/2} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1\,j} \\ x_{1j} & \cdots & x_{i-1\,j} & a_{jj} \end{vmatrix}^{1/2}}
$$

$$
= \frac{(a_{11})^{\frac{n-3}{2}}}{\sqrt{a_{22} \ldots a_{nn}}} \frac{\prod_{i=2}^{n-1} \begin{vmatrix} a_{11} & \cdots & x_{1\,i} \\ \vdots & \ddots & \vdots \\ x_{1\,i} & \cdots & a_{ii} \end{vmatrix}^{\frac{n-i-2}{2}}}{\prod_{2 \le i < j \le n} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1\,j} \\ x_{1j} & \cdots & x_{i-1\,j} & a_{jj} \end{vmatrix}^{\frac{1}{2}}}.
$$

Let i and j be integers, such that $2 \le i < j \le n$. Consider the matrix

$$
(4) \qquad \mathbf{M} = \begin{pmatrix} a_{11} & \cdots & x_{1i} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1i} & \cdots & a_{ii} & x_{ij} \\ x_{1j} & \cdots & x_{ij} & a_{jj} \end{pmatrix}.
$$

Applying the Sylvester's determinant identity (see [2], p.3) on the matrix $\mathbf{M}$ we get

(5)
$$|\mathbf{M}|\begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} \\ \vdots & \ddots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} \end{vmatrix} = \begin{vmatrix} a_{11} & \cdots & x_{1\,i} \\ \vdots & \ddots & \vdots \\ x_{1\,i} & \cdots & a_{ii} \end{vmatrix} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1j} \\ x_{1j} & \cdots & x_{i-1j} & a_{jj} \end{vmatrix} - \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1i} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1i} \\ x_{1j} & \cdots & x_{i-1\,j} & x_{ij} \end{vmatrix}^2 .$$

The last determinant in (5) can be written in the form

(6)
$$\begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1i} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1\,i} \\ x_{1j} & \cdots & x_{i-1\,j} & x_{ij} \end{vmatrix} = \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1i} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1\,i} \\ x_{1j} & \cdots & x_{i-1\,j} & 0 \end{vmatrix} + x_{ij} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} \\ \vdots & \ddots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} \end{vmatrix}.$$

From (3), (5) and (6) it follows that for $2 \le i < j \le n$

(7)
$$1 - y_{ij}^2 = \frac{\begin{vmatrix} a_{11} & \cdots & x_{1\,i} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i} & \cdots & a_{ii} & x_{ij} \\ x_{1j} & \cdots & x_{ij} & a_{jj} \end{vmatrix} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} \\ \vdots & \ddots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} \end{vmatrix}}{\begin{vmatrix} a_{11} & \cdots & x_{1\,i} \\ \vdots & \ddots & \vdots \\ x_{1\,i} & \cdots & a_{ii} \end{vmatrix} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1\,j} \\ x_{1j} & \cdots & x_{i-1\,j} & a_{jj} \end{vmatrix}}.$$

Therefore the joint density of the random variables $\nu_{ij},\ 1 \le i < j \le n$ is

$$g_{\nu_{ij},1\le i<j\le n}\left(x_{ij},\ 1 \le i < j \le n\right) = K_n \prod_{j=2}^{n} \left(1 - \frac{x_{1j}^2}{a_{11}a_{jj}}\right)^{\frac{n-2}{2}}$$

$$\times \prod_{2\le i<j\le n} \left[\frac{\begin{vmatrix} a_{11} \cdots x_{1\,i} & x_{1j} \\ \vdots \ \ddots \ \vdots & \vdots \\ x_{1\,i} \cdots a_{ii} & x_{ij} \\ x_{1j} \cdots x_{ij} & a_{jj} \end{vmatrix} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} \\ \vdots & \ddots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} \end{vmatrix}}{\begin{vmatrix} a_{11} \cdots x_{1\,i} \\ \vdots \ \ddots \ \vdots \\ x_{1\,i} \cdots a_{ii} \end{vmatrix} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1j} \\ x_{1j} & \cdots & x_{i-1\,j} & a_{jj} \end{vmatrix}} \right]^{\frac{n-i-1}{2}} |\mathbf{J}|\, I_{S'} = \frac{K_n}{(a_{11}a_{22}\dots a_{nn})^{\frac{n-1}{2}}} I_{S'}.$$

It remains to prove that $I_S' \equiv I_S$. This follows immediately from the next Lemma.

Lemma 1. *The matrix* **A** *in (2) is positively definite if and only if*

$$a_{ii} > 0, \quad i = 1, \ldots, n;$$

$$\frac{\begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1i} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1\,i} \\ x_{1j} & \cdots & x_{i-1\,j} & 0 \end{vmatrix} + x_{ij} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} \\ \vdots & \ddots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} \end{vmatrix}}{\begin{vmatrix} a_{11} & \cdots & x_{1\,i} \\ \vdots & \ddots & \vdots \\ x_{1\,i} & \cdots & a_{i\,i} \end{vmatrix}^{1/2} \begin{vmatrix} a_{11} & \cdots & x_{1\,i-1} & x_{1j} \\ \vdots & \ddots & \vdots & \vdots \\ x_{1\,i-1} & \cdots & a_{i-1i-1} & x_{i-1\,j} \\ x_{1j} & \cdots & x_{i-1\,j} & a_{jj} \end{vmatrix}^{1/2}} \in (-1,\, 1),$$

$i = 2, \ldots, n-1,\ j = i+1, \ldots, n.$

The proof of the Lemma in the case $a_{11} = a_{22} = \cdots = a_{nn} = 1$ is given in [4]. In the general case the proof is based on the fact that the matrix **A** may be written as

$$\mathbf{A} = \mathbf{DBD},$$

where **D** is the diagonal matrix $\mathbf{D} = \operatorname{diag}(\sqrt{a_{11}}, \sqrt{a_{22}}, \ldots, \sqrt{a_{nn}})$ and **B** is a matrix with units on the main diagonal. Moreover matrix **A** is positively definite if and only if matrix **B** is. The detailed proof of the Lemma will appear in a forthcoming publication.

Theorem 2. *Relation (1) can be written in the form:*

$$\text{(8)} \quad \nu_{ij} = \sqrt{a_{ii}a_{jj}} \left[\sum_{k=1}^{i-1} \left(\eta_{ki}\eta_{kj} \prod_{s=1}^{k-1} \sqrt{(1-\eta_{si}^2)(1-\eta_{sj}^2)} \right) + \eta_{ij} \prod_{s=1}^{i-1} \sqrt{(1-\eta_{si}^2)(1-\eta_{sj}^2)} \right]$$
$$i = 2, \ldots, n-1, \quad j = i+1, \ldots, n$$

Proof. We give here the main ideas of the proof. The whole proof will appear in a forthcoming publication.

For any integers k and s, $1 < k < s \leq n$ it can be seen by (7) that

$$\text{(9)} \quad \left(\prod_{1 \leq i < j \leq k} (1-\eta_{ij}^2) \right) \left(\prod_{i=1}^{k} (1-\eta_{is}^2) \right) = \frac{1}{a_{11} \ldots a_{kk} a_{ss}} \begin{vmatrix} a_{11} & \cdots & \nu_{1\,k} & \nu_{1s} \\ \vdots & \ddots & \vdots & \vdots \\ \nu_{1\,k} & \cdots & a_{kk} & \nu_{ks} \\ \nu_{1s} & \cdots & \nu_{ks} & a_{ss} \end{vmatrix}.$$

By induction on r it can be proved that for any integer r,k and s, $1 < r < k < s \leq n$

$$\text{(10)} \quad \begin{vmatrix} a_{11} & \cdots & \nu_{1r} & \nu_{1k} \\ \vdots & \ddots & \vdots & \vdots \\ \nu_{1r} & \cdots & a_{rr} & \nu_{rk} \\ \nu_{1s} & \cdots & \nu_{rs} & 0 \end{vmatrix} =$$
$$-a_{11} \ldots a_{rr} \sqrt{a_{ss}a_{kk}} \left(\prod_{1 \leq i < j \leq r} (1-\eta_{ij}^2) \right) \sum_{i=1}^{r} \left(\eta_{ik}\eta_{is} \prod_{j=1}^{i-1} \sqrt{(1-\eta_{jk}^2)(1-\eta_{js}^2)} \right).$$

Now, applying (9) and (10) to (1) it is easy to get representation (8), which completes the proof.

Theorems 1 and 2 give the following algorithm for generating random uniformly distributed positively definite matrices:

1) Generate $n(n-1)/2$ random numbers y_{ij}, $1 \le i < j \le n$ so that y_{ij} comes from the distribution $\Psi(n-i)$.

2) In order to reduce calculations, compute the auxiliary quantity z_{ij}, $1 \le i \le j \le n$ such that

$$z_{ij} = y_{ij}\sqrt{(1-y_{1j}^2)\dots(1-y_{i-1j}^2)} \text{ with } y_{ii} = 1.$$

3) Calculate the desired matrix (2) with

$$x_{ij} = \sqrt{a_{ii}a_{jj}}(z_{1i}z_{1j} + z_{2i}z_{2j} + \dots + z_{ii}z_{ij}).$$

The obtained formulas show that it is possible to create a program, which generates without dialog with the user a matrix $\mathbf{U}$ with units on the main diagonal. This is done in steps 1)-3) substituting $a_{11} = \dots = a_{nn} = 1$. Then the user, according to his preferences, form a diagonal matrix $\mathbf{D} = \operatorname{diag}(\sqrt{a_{11}}, \dots, \sqrt{a_{nn}})$ and the desired matrix $\mathbf{A}$ is

$$\mathbf{A} = \mathbf{DUD}.$$

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ГЕНЕРИРАНЕ НА РАВНОМЕРНО РАЗПРЕДЕЛЕНИ ПОЛОЖИТЕЛНО ОПРЕДЕЛЕНИ МАТРИЦИ

Евелина И. Велева

В тази статия са разгледани статистики, които имат съвместно равномерно разпределение върху множество от всички положително определени матрици с предварително фиксирани диагонални елементи. Това ни дава алгоритъм за генериране на случайни положително определени матрици с равномерно разпределение.