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THE GENERATION OF A RANDOM SAMPLE-COVARIANCE MATRIX

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Houston, Texas

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ABSTRACT

In simulating trajectory estimation problems, a rapid procedure is desirable for generating random sample-covariance matrices based on large numbers of observations. By using existing random-number generators, an economical method is developed that yields a matrix S^* whose elements have the same joint distribution as the elements of the sample-covariance matrix S.

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SUMMARY

Trajectory estimation simulation problems make desirable a rapid procedure for generating random sample-covariance matrices based on large numbers of observations. This paper first presents an algorithm for such a procedure and then shows its derivation from the Cochran-Fisher Theorem concerning quadratic forms. Finally, an example is given.

INTRODUCTION

In trajectory analysis, the "best" estimate of the state is a function of the covariance matrices R_i associated with the observation stations. For practical use, estimates must be substituted for the unknown exact R_i. In some cases, estimating the R_i directly from the observations may be desirable.

The well-known "best", or unbiased-maximum-likelihood-based (u.m.l.b.), estimator of a covariance matrix R_i is given by

$$S = \frac{1}{n - 1} \sum_{i=1}^{n} \left(X_i - X\right)\left(X_i - X^T\right) \tag{1}$$

where the X_i are the observation vectors and n is the sample size. To simulate a procedure where u.m.l.b. estimates are used, random matrices must be generated that have the same distribution as these estimates.

The obvious method of generating a matrix S^*, having the same distribution as S, is to generate the n observation vectors $\left\{X_i; \ i = 1, \ldots n\right\}$. But if each vector X_i has p components, generating n observation vectors necessitates generating at least np random numbers.

This paper presents an alternate method of generating S^* which requires using only $p(p + 1)/2$ random numbers - usually a much smaller quantity than np.

SYMBOLS

$A, A^*, B, B^*, C, R, W, S, S^*$	matrices
A_i	matrices in Cochran's Theorem
b_{ij}	ij^{th} element of B
b^*_{ij}	ij^{th} element of B^*
C^T	transpose of the matrix C
I	identity matrix
i, j, k	indices of summation
$N(\emptyset,R)$	normally distributed with mean $\emptyset$ and covariance matrix R
N_j, N_{ij}	standardized normal random variates
n	sample size
p	size of covariance matrix (number of variables in one observation)
Q	matrix equal to $I - \sum_{k=1}^{j-1} Q_k$
Q_i	matrix equal to $y_i^T y_i / y_i y_i^T$
r_j	j^{th} row of matrix W
r_j^T	transpose of r_j

t_k^T	transpose of t_k
v_j	random variable
w_{ij}	ij^{th} element of W
x	$1 \times (n - 1)$ random vector in Cochran's Theorem
y_j	j^{th} of a set of orthogonal $1 \times (n - 1)$ vectors
y_j^T	transpose of y_j
z_k, t_k	$p \times 1$ vectors
$\chi^2 (n - j)$	chi-square with $n - j$ degrees of freedom
ν_i	rank of A_i
$\emptyset$	$p \times 1$ null vector
$\sim$	is distributed as

METHOD

Let $S = A/(n - 1)$ be the u.m.l.b. estimator of a $p \times p$ covariance matrix R from an independent normally distributed sample of size n. It can be shown (ref. 1) that

$$A = \sum_{k=1}^{n-1} z_k z_k^T \tag{2}$$

where the $p \times 1$ vectors $\{z_k;\ k = 1, 2, \ldots n - 1\}$ are independent and normally distributed with zero mean and covariance matrix R.

Since R is a covariance matrix, it is semipositive definite. Therefore, a matrix C exists such that

$$CC^T = R \tag{3}$$

It follows that the vector z_k can be written

$$z_k = Ct_k \tag{4}$$

where

$$t_k \sim N(\emptyset, I)$$

Let

$$B = \{b_{ij}\} = \sum_{k=1}^{n-1} t_k t_k^T \tag{5}$$

Then,

$$CBC^T = C \sum_{k=1}^{n-1} t_k t_k^T C^T = A \tag{6}$$

Generation of A^*

Let A^* be a generated matrix whose elements have the same joint distribution as those of A. To obtain $S^* = A^*/(n - 1)$, it is necessary only to generate a matrix B^* whose elements are distributed as the elements of B. Then, A^* is computed so that

$$A^* = CB^*C^T \tag{7}$$

Hence, the problem is reduced to generating the random symmetric matrix B^*. An algorithm for generating B^* is given below. For a justification of this procedure, refer to the Analysis.

Generation of B^*

1. Generate p independent χ^2 variables v_j, $j = 1,\ldots p$, having $n - j$ degrees of freedom. One method of obtaining v_j is to generate a standard normal variate N_j and substitute it into the Wilson-Hilferty χ^2 approximation (ref. 2). The approximation can be written

$$v_j \approx (n - j)\left[1 - \frac{2}{9\,(n - j)} + N_j\sqrt{\frac{2}{9\,(n - j)}}\right]^3$$

2. Generate $p(p - 1)/2$ independent standard normal variates N_{ij}, $i < j$, and $j = 1, 2, \ldots p$.

3. Form the diagonal elements of $B^*\left(b^*_{jj},\ j = 1, \ldots p\right)$ as follows:

$$b^*_{11} = v_1$$

$$b^*_{jj} = v_j + \sum_{i=1}^{j-1} N_{ij}^{\,2} \quad (j > 1)$$

4. Form the off-diagonal elements of B^* as follows:

$$b^*_{1j} = b^*_{j1} = N_{1j}\sqrt{v_1}$$

$$b^*_{ij} = b^*_{ji} = N_{ij}\sqrt{v_i} + \sum_{k=1}^{i-1} N_{ki}N_{kj} \quad (i > 1)$$

Once B^* has been generated, A^* follows from equation (7).

ANALYSIS

Using the notation of the Method section and noting that by joining the vectors t_k and $k = 1, 2, \ldots n - 1$ as columns, a $p \times (n-1)$ matrix W can be formed

$$W = \left\{w_{ij}\right\} = \left(\begin{bmatrix} t_1 \end{bmatrix} \begin{bmatrix} t_2 \end{bmatrix} \cdots \begin{bmatrix} t_{n-1} \end{bmatrix} \right) = \begin{pmatrix} \begin{bmatrix} r_1 \end{bmatrix} \\ \begin{bmatrix} r_2 \end{bmatrix} \\ \vdots \\ \begin{bmatrix} r_p \end{bmatrix} \end{pmatrix}$$

where r_j is the j^{th} $1 \times (n - 1)$ row vector of W. Thus, the ij^{th} element of B, b_{ij}, is equal to $r_i r_j^T$.

By using the Schmidt orthogonalization process, a set of orthogonal vectors $\{y_j, \; j = 1, 2, \ldots p\}$ can be generated where

$$\begin{aligned} y_j &= r_j - r_j y_1^T y \Big/ y_1 y_1^T - \cdots r_j y_{j-1}^T y_{j-1} \Big/ y_{j-1} y_{j-1}^T \\ &= r_j \left(I - Q_1 - Q_2 - \cdots Q_{j-1} \right) \\ &= r_j Q \end{aligned} \tag{8}$$

where $Q_i = y_i^T y_i \Big/ y_i y_i^T$, $Q = I - \sum_{k=1}^{j-1} Q_k$ and I is the $(n - 1) \times (n - 1)$ identity matrix.

The matrices $Q, Q_1, \ldots Q_{j-1}$ have the following significant properties:

1. $Q_1, Q_2, \ldots Q_{j-1}$ have a rank of one.

2. $Q_i Q_j = 0$ for $i \neq j$.

3. $Q, Q_1, \ldots Q_{j-1}$ are symmetric idempotents.

4. Q has rank $n - j$.

Proof

1. The vector y_i clearly spans the entire range space of Q_i.

2. $$Q_i Q_j = \frac{y_i^T y_i y_j^T y_j}{\left(y_i y_i^T\right)\left(y_j y_j^T\right)} = 0 \text{ because } y_i y_j^T = 0 \text{ for } i \neq j.$$

3. Clearly Q_i is symmetric. To show idempotence,

$$Q_i Q_i = \frac{y_i^T \left(y_i y_i^T \right) y_i}{\left(y_i y_i^T\right) \left(y_i y_i^T\right)} = \frac{y_i^T y_i}{y_i y_i^T} = Q_i$$

and

$$\begin{aligned} QQ &= \left(I - Q_1 - \dots Q_{j-1}\right)\left(I - Q_1 - \dots Q_{j-1}\right) \\ &= I - 2\left(Q_1 + \dots Q_{j-1}\right) + \left(Q_1 + \dots Q_{j-1}\right) \\ &= I - \left(Q_1 + \dots Q_{j+1}\right) = Q \end{aligned}$$

4. This follows from elementary theorems on idempotent matrices (ref. 3). Consider the following form of the Cochran-Fisher Theorem.

Theorem

If x *is a* $1 \times (n - 1)$ *random vector distributed* $N(\emptyset, I)$, *and if* $xx^T = \sum_{i=1}^{k} xA_i x^T$ *the rank of the sum of the* A_i's *equalling the sum of the ranks of the separate* A_i's *is a necessary and sufficient condition for* $xA_i x^T$ *to be distributed as central* χ^2 *with* ν_i *degrees of freedom* $\left(\text{where } \nu_i \text{ is the rank of } A_i\right)$, *and for* xA_1x^T, xA_2x^T, $\dots$ xA_kx^T *to be jointly independent* (ref. 4).

Note that the inner product $r_j r_j^T$ can be written

$$r_j r_j^T = r_j I r_j^T = r_j \left(Q + Q_1 + \dots Q_{j-1} \right) r_j^T$$

$$= r_j Q r_j^T + \sum_{k=1}^{j-1} r_j Q_k r_j^T \tag{9}$$

Equation (9) satisfies the condition of the Theorem where the matrices Q, Q_1, ... Q_{j-1} play the role of the A_i. It therefore follows that

$$r_j Q r_j^T = r_j Q Q^T r_j^T = r_j Q \left(r_j Q \right)^T = y_j y_j^T \sim \chi^2 (n - j)$$

Since the y_j are mutually orthogonal and normally distributed, the quantities $y_j y_j^T$, $(j = 1, 2, \dots p)$, are mutually independent. They can be generated independently using random variables v_j, having the χ^2 distribution with $n - j$ degrees of freedom.

Once the set $\left\{ y_j y_j^T, \; j = 1 \dots p \right\}$ is given, the quantities

$$\sigma_{ij} = \left(r_j Q_i r_j^T \right)^{1/2} = \left(\frac{r_j y_i^T y_i r_j^T}{y_i y_i^T} \right)^{1/2} = \frac{r_j y_i^T}{\left(y_i y_i^T \right)^{1/2}} \tag{10}$$

being normalized linear combinations of $N(0,1)$ variates, are themselves, $N(0,1)$ variates.

Since all the elements of the matrix W are mutually independent, σ_{ij} is independent of $\sigma_{i'j'}$ for $j \neq j'$, $i < j$, $i' < j'$. Furthermore, as a consequence of the Theorem, it is known that for $i \neq i'$, σ_{ij} is independent of $\sigma_{i'j}$. Therefore, the $p(p + 1)/2$ quantities, $y_j y_j^T$ and $\sigma_{ij}(j = 1, p; i < j)$, can be generated independently, using the χ^2 random variable v_j for $y_j y_j^T$ and standardized normal variates N_{ij}, for σ_{ij}.

The diagonal elements of B^* are easily computed from equation (9). Let

$$b^*_{11} = v_1$$

$$b^*_{jj} = v_j + \sum_{i=1}^{j-1} N_{ij}^2 \quad (j > 1)$$

Since $\sigma_{ij} \sqrt{y_i y_i^T} = r_j y_i^T$, it follows that

$$N_{ij} \sqrt{v_i} \sim r_j y_i^T$$

From equation (7) for $i < j$,

$$r_j y_i^T = r_j \left[r_i^T - \frac{\left(r_i y_1^T\right)}{\left(y_1 y_1^T\right)} y_1^T - \frac{\left(r_i y_2^T\right)}{\left(y_2 y_2^T\right)} y_2^T - \cdots \frac{\left(r_i y_{i-1}^T\right)}{\left(y_{i-1} y_{i-1}^T\right)} y_{i-1}^T \right]$$

$$\sim r_j r_i^T - \left[\frac{N_{1i}}{\sqrt{v_1}} \left(r_j y_2^T\right) + \frac{N_{2i}}{\sqrt{v_2}} \left(r_j y_2^T\right) + \cdots \frac{N_{i-1i}}{\sqrt{v_{i-1}}} \left(r_j y_{i-1}^T\right) \right]$$

$$\sim b_{ji} - \left(N_{1i} N_{1j} + N_{2i} N_{2j} + \cdots N_{i-1i} N_{i-1j}\right)$$

Therefore, $b^*_{ij} = b^*_{ji}$ can be generated by

$$b^*_{ij} = N_{ij} \sqrt{v_1}$$

$$b^*_{ij} = N_{ij} \sqrt{v_i} + \sum_{k=1}^{i-1} N_{ki} N_{kj} (i - 1).$$

Example

Consider the generation of S^* based on 101 observations when R is given to be $\begin{bmatrix} .45 & -.21 & 0 \\ -.21 & .50 & .05 \\ 0 & .05 & .25 \end{bmatrix}$

Then $n = 101$, $p = 3$, and $C = \begin{bmatrix} .6 & -.3 & 0 \\ 0 & .7 & .1 \\ 0 & 0 & .5 \end{bmatrix}$

It is necessary to generate only 6 (instead of 606) random numbers from an $N(0,1)$ population. They are:

$$N_1 = -0.258 \qquad N_{12} = -0.585$$

$$N_2 = -0.882 \qquad N_{13} = 0.332$$

$$N_3 = 1.869 \qquad N_{23} = -0.110$$

The Wilson-Hilferty χ^2 approximation gives:

$$v_1 = 100 \left[1 - \frac{2}{(9)(100)} + \frac{(-0.238)\sqrt{2}}{\sqrt{900}} \right]^3 = 96.027$$

$$v_2 = 99 \left[1 - \frac{2}{(9)(99)} + \frac{(-0.882)\sqrt{2}}{\sqrt{891}} \right]^3 = 86.492$$

$$v_3 = 98 \left[1 - \frac{2}{(9)(98)} + \frac{(-1.869)\sqrt{2}}{\sqrt{882}} \right]^3 = 125.769$$

Finally, the procedure given in the Method section yields

$$b^*_{11} = 96.027$$

$$b^*_{22} = 86.492 + (-0.585)^2 = 86.835$$

$$b^*_{33} = 125.769 + (0.332)^2 + (-0.110)^2 = 125.891$$

$$b^*_{12} = -0.585\sqrt{96.027} = -5.734$$

$$b^*_{13} = 0.332\sqrt{96.027} = 3.250$$

$$b^*_{23} = -0.110\sqrt{86.492} + (-0.585)(0.332) = -1.216$$

Thus,

$$A^* = C^T B^* C$$

$$= \begin{bmatrix} 44.449 & -20.412 & 1.157 \\ -20.412 & 43.638 & 5.869 \\ 1.157 & 5.869 & 31.473 \end{bmatrix}$$

and

$$S^* = A^*/(n - 1) = \begin{bmatrix} 0.444 & -0.204 & 0.012 \\ -0.204 & 0.436 & 0.059 \\ 0.012 & 0.059 & 0.315 \end{bmatrix}$$

CONCLUDING REMARKS

This report has presented an economical method of generating a $p \times p$ sample covariance matrix based on n observations. The method requires the generation of only $p(p + 1)/2$ random numbers instead of the usually much larger quantity np. The matrix C referred to in the Method section may be obtained by methods readily adaptable to computers.

Manned Spacecraft Center
National Aeronautics and Space Administration
Houston, Texas, October 18, 1965

REFERENCES

1. Anderson, T. W.: An Introduction to Multivariate Statistical Analysis. John Wiley and Sons, Inc., 1958, p. 53.

2. Wilson, E. B.; and Hilferty, M. M.: The Distribution of Chi-Square. Proc. Nat. Acad. Sci., USA 17, 1931, pp. 684-688.

3. Graybill, F. A.: An Introduction to Linear Statistical Models, Vol. 1. McGraw-Hill Book Co., Inc., 1961, pp. 16, 86.

4. Perlis, S.: Theory of Matrices. Addison-Wesley, 1952, p. 89.

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