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On Random Correlation Matrices II. The Toeplitz Case

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Lincoln Laboratory

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MASSACHUSETTS INSTITUTE OF TECHNOLOGY
LINCOLN LABORATORY

**ON RANDOM CORRELATION MATRICES
II. THE TOEPLITZ CASE**

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Group 32

TECHNICAL REPORT 816

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ABSTRACT

The problem of generating random Toeplitz correlation matrices is considered. Several methods are proposed, of which the most promising, as determined by both computational complexity and spectral randomness, seems to be that based on the characteristic function of random discrete probability measure. A number of interesting theoretical issues are recorded for further investigation. This report follows an earlier one devoted to general random correlation matrices. In both cases the intent is to use such matrices to simulate random data for the testing of certain group-theoretic signal processing algorithms.

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1. INTRODUCTION

The following is intended as a sequel to our earlier report on random correlation matrices [11]. All this work is ultimately motivated by eventual application to the testing and comparison of certain signal processing algorithms, specifically those defined by group transforms and filters, and intended for such second order tasks as data compression and decorrelation, and Wiener filtering. The earlier report, particularly its summary, contains further details on these applications.

The basic idea is that a random correlation matrix (RCM) is to be interpreted as the covariance matrix of a random, or ‘average,’ signal. The latter is conceived as a random vector, whose components all have an equal variance (here taken as unity). This vector arises, in turn, from sampling and quantizing a continuous signal. If the latter can be reasonably modeled as a stationary stochastic process, then the resulting covariance matrix of the samples will have a Toeplitz structure, that is, it will be Hermitian and have constant diagonals. Hence it can be fully specified by, for example, its first row.

Our view is that a Toeplitz random correlation matrix (TRCM) represents an intermediate degree of statistical structure between general random signals as described by RCMs, and signals describable as outputs of very special models, such as linear stochastic difference equations. The latter result in autoregressive signal models of some finite order m , denoted $AR(m)$. In our numerical studies of group - theoretic signal processing algorithms, we restrict to the cases $m \leq 2$. There is an interesting cluster of theoretical questions here, pertaining to the density of such signals and their matrices, which will be listed later in Section 4, along with other unresolved issues.

The specific problem which we address below is that of generating TRCMs. As in the earlier report, we distinguish two aspects of this problem: analytical and computational. The latter refers to computer software whose implementation results in an output stream of pseudorandom TRCMs. We will also have a few remarks to make about some spectral distributions associated with our TRCMs, but not to the extent of those in [11]; most of the natural questions in this context are left to Section 4.

The general topic of Toeplitz matrices and operators is extensively developed by now, and in no way encompassed by a few sources. Some general references are the books [10, 12] and articles [9, 19], but these already provide more background than is really necessary for present purposes.

The subject of random correlation matrices as presented in this and the preceding report [11], and in several references listed there, is but one aspect of the much larger area of *random matrices*. As we see it, this area encompasses, in addition to the present topic, the asymptotics of the spectral distributions of large random matrices, given distributional information about the matrix entries, and the problem of sampling from various compact matrix groups (symmetric groups, orthogonal groups, etc.). Collectively, random matrix theory has a vast array of applications in the sciences (nuclear physics, biology), communications engineering (coding, encryption), statistics (simulation, projection pursuit, algorithm tests), and mathematics (random walks, spectral asymptotics, ergodic theory). The recent conference proceedings [16] gives an overview of many of these applications, along with considerable theory. The books [3, 18] give, respectively, a physical and a mathematics

perspective on random matrices, with emphasis on eigenvalue distributions. For the early work, emanating from the need to statistically model energy levels of complex nuclei, dating at least from E. Wigner (1957), see his survey article [21]. Finally, there are two Russian books by V. Girko (Kiev, 1975 and 1980) on random matrices and random determinants, respectively, which have not been available to the author.

2. THE METHODS

In this section we will discuss five possible methods for defining TRCMs. The first, an attempt at extending the random Gram method of [11] for generating RCMs, is rejected as being infeasible. The second method, derived from the well-known structure of moving average processes, is simple and efficient, and was our initial choice. The third, which builds up a matrix from the characteristic function of a random probability distribution, is the most interesting theoretically, it can be reasonably efficient, and can give good spectral distribution properties, at least for small matrix size. The remaining two have various deficiencies of both a theoretical and practical nature that probably render them unsuitable for automatic use. Yet each of them involves interesting open questions, and thus it is felt that they are worthy of brief mention in the present context.

Before detailing the five methods, let us be specific about what we are trying to do. For a fixed positive integer N we want a procedure for producing a stream of $N \times N$ matrices of the form

$$\begin{bmatrix} 1 & a & b & \dots & c \\ \bar{a} & 1 & a & \dots & \\ \bar{b} & \bar{a} & 1 & & \\ \vdots & & & \dots & a \\ \bar{c} & \dots & \dots & \bar{a} & 1 \end{bmatrix}, \quad (2.1)$$

each of which is, in addition, positive definite. The $N-1$ free entries a, b, \dots are to be deterministic functions of some random variables. In the real symmetric case, of course, we will have $a = \bar{a}$, $b = \bar{b}$, \dots , etc. For computer implementation we will expect to be able to reduce all randomness to pseudorandom samples from the univariate uniform or normal distributions. Any matrix of the form (2.1) constructed by some such procedure is by definition a TRCM.

Method 1 This is based on the procedure extensively discussed in [11]. That procedure yields what were called there random Gram matrices. Namely, for fixed N , we select N random vectors v_1, \dots, v_N independent and uniformly distributed on the unit sphere in the real space of N (or more) dimensions, and form the Gram matrix

$$A = [\langle v_i, v_j \rangle]. \quad (2.2)$$

General theory forces A to be almost surely positive definite and hence A is a correlation matrix, since

$$\langle v_i, v_i \rangle = \|v_i\|^2 = 1, \quad i = 1, \dots, N.$$

Extension of this method to the present Toeplitz case then reduces to the question of whether this further symmetry can be attained by some geometrical constraints on the mutual position of the vectors v_i . For example, in the $N = 3$ case, we would choose v_1, v_3 independent, and then v_2 at

random from the unit sphere in the plane $(v_1 - v_3)^\perp$. This would guarantee that $\langle v_1, v_2 \rangle = \langle v_2, v_3 \rangle$, and hence that the Gram matrix A in Equation (2.2) is Toeplitz. With a little more effort an analogous procedure could be developed for the $N = 4$ case, but we have not been able to obtain such an algorithm for general N .

Method 2 This is based on the well-known formula for the autocorrelation function of a (stationary) moving average process. If $\{x_t\}$ is such a process, of order p , then there are constants $c_0 = 1, c_1, \dots, c_p$, such that $x_t = w_t + c_1 w_{t-1} + \dots + c_p w_{t-p}$, where $\{w_t\}$ is a white noise process. It follows that

$$\text{cov}(x_{t+k}, x_t) = \sigma^2 \sum_{j=0}^{p-|k|} c_j c_{j-|k|}, \quad (2.3)$$

for $|k| \leq p$, and 0 otherwise. Here σ^2 is the variance of the noise terms w_t ; we may as well take $\sigma = 1$ for present purposes. The function of k defined by Equation (2.3) is the autocorrelation function of the process $\{x_t\}$, up to normalization by the factor $(1 + c_1^2 + \dots + c_p^2)$, and, as such, is in particular a positive definite function on the group \mathbb{Z} of integers.

Now, by definition, this property of a function ϕ defined on \mathbb{Z} is exactly that required for the matrix A defined by

$$A = [\phi(i - j)], \quad (2.4)$$

to be a Toeplitz covariance matrix. Hereafter we will enforce the normalization $\phi(0) = 1$, so that A is actually a correlation matrix. So, at this point we may say that a normalized positive definite function on \mathbb{Z} will give rise to a Toeplitz correlation matrix of any order through the prescription of Equation (2.4), and that, for a fixed order, a simple way to obtain such functions is through the covariance formula (2.3).

With this background we can now state a simple algorithm for generating real TRCMs:

- Select matrix dimension N ;
- Generate a vector (x_1, \dots, x_N) from the uniform distribution on the unit sphere in \mathbb{R}^N ;
- Define a function ϕ on \mathbb{Z}^+ by $\phi(k) = \sum_{j=1}^N x_j x_{j+k}$ with the convention that $x_j = 0, j > N$;
- Define the associated correlation matrix C by $C = [\phi(|i - j|)]$.

We note that procedures for carrying out Step 2 above are discussed in [11, Section 5.1] and, in greater depth, in [6, Section 5.4]. Some spectral properties of this method are given in the next section.

Method 3 We continue with the theme of using positive definite functions to generate Toeplitz correlation matrices according to Equation (2.4). Hence we will permit an interest in generating complex Hermitian Toeplitz correlation matrices, as displayed in Equation (2.1). (If real Toeplitz correlation matrices are required, then the real parts of the eventual complex matrices may be taken; doing so will not alter the spectrum.) For this it is sufficient to have a procedure for generating positive definite functions on the group \underline{R} of real numbers. Of course, there is a slight case of ‘overkill’ in this approach since such a function ϕ will produce infinitely many matrices of the desired sort, and of any dimension N , by the formula

$$C = [\phi(t_i - t_j)], \quad (2.5)$$

where $\{t_i\} \subset \underline{R}, i, j = 1, \dots, N$, and we would want the work required to specify ϕ to be somehow scaled to the size of N .

We make use of Bochner’s theorem which states that each continuous normalized positive definite function is the characteristic function of a probability distribution on \underline{R} . That is

$$\phi(x) = \int_{\underline{R}} e^{ixt} dP(t), \quad (2.6)$$

where $P(\bullet)$ is a distribution function on \underline{R} , or, equivalently, a probability measure on (the Borel subsets of) \underline{R} . Hence, via the correspondence $P \rightarrow \phi \rightarrow C$, we see that a method for generating TRCMs will follow from any method that randomly selects a probability measure P on \underline{R} .

Such a method would seem to involve us with the concept of a probability measure over the (enormous!) space $\Pi(\underline{R})$ of all probability measures on \underline{R} . In fact, such measures have been introduced in the context on nonparametric Bayesian statistical analysis by T. Ferguson in 1973-74, and termed Dirichlet processes. (Actually, the concept of a random probability measure with fixed, bounded support, e.g., $[0, 1]$, identified with the corresponding distribution function, goes back at least 10 years earlier [7].) To engage in a substantial discussion of these would constitute a further case of ‘overkill’ in the present context. So let us just say that Dirichlet processes can be parameterized by the set of finite measures on \underline{R} , that is, measures of the form $\beta = t\rho, t > 0, \rho \in \Pi(\underline{R})$. If D_β is the Dirichlet process corresponding to such a β , then for any partition $\underline{R} = B_1 \cup \dots \cup B_k$, the random vector $[D_\beta(B_1), \dots, D_\beta(B_k)]$ has the Dirichlet distribution with parameters $(\beta(B_1), \dots, \beta(B_k))$. In particular, we can say that $E(D_\beta) = \rho (= t^{-1}\beta)$. A basic survey article is [8] with other early work by C. Antoniak, D. Blackwell, and J. MacQueen. There have been sporadic developments since then associated with such authors as S. Dalal, J. Sethuramen, R. Tiwari, *inter alia*. Some of this work involves the concept of an exchangeable sequence of random variables.

One key result due independently to several of the early authors is that a $\rho \in \Pi(\underline{R})$ chosen at random from a Dirichlet process is almost surely discrete. A particularly nice constructive specification of a Dirichlet process was given in [2]. It is based on abstract ‘Polya urn scheme’ (drawing balls of various colors from an urn, with a prior distribution on the colors; infinitely many colors allowed), and yields approximating measures of the form

$$\mu_N = c_N^{-1}(\beta + \delta(t_1) + \dots + \delta(t_N)), \quad (2.7)$$

with $c_N = \beta(\underline{R}) + N$, and $\delta(t) =$ the point measure concentrated at $t\varepsilon\underline{R}$. It is clear that such measures could be rather easily simulated on a computer. From there, the resulting μ_N is substituted for P in Equation (2.6), thereby defining the function ϕ which, in turn, is used in Equation (2.5) to define a Toeplitz correlation matrix C (with some particular choice of points t_i).

We have not carried out this program although it appears to be a very interesting project, particularly because of the likely theoretical relationships between various spectral properties of the resulting TRCMs and the probabilistic structure of the random measures μ_N that might thereby be suggested.

Instead, we offer the following *ad hoc* algorithm for generating a discrete random probability measure P , which is then used in the usual way to define a Toeplitz correlation matrix:

- Select matrix dimension N ;
- Select an integer $L > N$, and a positive number σ ;
- Generate a random point (p_1, \dots, p_L) from the unit simplex, so that $p_i > 0$, $\sum p_i = 1$;
- Generate a random point (s_1, \dots, s_L) from the centered multivariate normal distribution with $L \times L$ covariance matrix $= \sigma^2 I_L$;
- Define $P = p_1\delta(s_1) + \dots + p_L\delta(s_L)$;
- Define ϕ from Equation (2.5), and finally C from Equation (2.4) with $t_i = i$ there.

The choice of the integer L in the second step above is important, as too large or too small a value causes a distinctly nonrandom distribution of eigenvalues. From our numerical work reported in the next section, it appears that $L = 3N$ is a good choice. Note that $L \geq N$ is necessary for positive definiteness of C . The choice of σ is less crucial; $\sigma \in [5N, 10N]$ seems to be effective.

A procedure for carrying out the third step above was discussed in [11, Section 4.1]; it reduces to taking p_i to be the i th spacing in a sample of size $L - 1$ from the standard uniform $U[0, 1]$ distribution.

Method 4 This is based in the geometric notion of orthogonal projection in matrix space. We consider, in the real or complex case respectively, the real ordered vector space of real symmetric or complex Hermitian $N \times N$ matrices. Let us call this space X_N and denote its linear subspace of all Toeplitz matrices of the form (2.1) by T_N . Equipped with the usual Hilbert - Schmidt inner product

$$\langle A, B \rangle = \text{tr}(AB^*), \quad (2.8)$$

X_N becomes a real Hilbert space, and we can contemplate the operation of orthogonal projection of X_N onto the subspace T_N . Let us denote this operation by

$$A \rightarrow A_T, \quad A \in X_N. \quad (2.9)$$

It turns out to be easy to compute this projection because of the presence of an obvious orthogonal basis for T_N . Namely, if we specify a Toeplitz symmetric or Hermitian matrix by giving its first row, then the basis is given by the standard unit vector basis for \underline{R}^N in the real case, and these vectors plus $\sqrt{-1}$ times these vectors in the complex case (omitting $(1, 0, \dots, 0)^t$ in this case). Thus

$$\dim(T_N) = \begin{cases} N, & \text{real case} \\ 2N - 1, & \text{complex case.} \end{cases}$$

If we examine the nature of the projection operation by computing the Fourier coefficients of a matrix in X_N , A_T is obtained by averaging each diagonal. Thus, for instance, if $N = 4$, and

$$A = \begin{bmatrix} a & e & h & l \\ & b & f & k \\ & & c & g \\ & & & d \end{bmatrix},$$

then

$$A_T = \begin{bmatrix} \alpha & \beta & \gamma & \delta \\ & \alpha & \beta & \gamma \\ & & \alpha & \beta \\ & & & \alpha \end{bmatrix},$$

with $\alpha = (a + b + c + d)/4$, $\beta = (e + f + g)/3$, $\gamma = (h + k)/2$, and $\delta = l$.

It follows that if we start with a correlation matrix $C \in X_N$, its Toeplitz projection C_T will again be a correlation matrix, provided that it has no negative eigenvalues. Unfortunately, this need not be the case. Table 2-1 below exhibits for $N = 4, 5$, correlation matrices in X_N , their Toeplitz projections, and a negative eigenvalue for each of the latter. Thus we cannot conclude that a correlation matrix necessarily projects onto a Toeplitz correlation matrix (surprisingly, however, we were unable to find a counterexample for $N = 3$).

In spite of this somewhat disappointing discovery, an interesting empirical phenomenon occurs in this context, one that seems worthy of further investigation and explanation. Namely, the empirical frequency of the outcome (correlation matrix with indefinite Toeplitz projection) tends rather rapidly to 0 with increasing values of N . Evidence for this statement is summarized in Table 2-2 below. The underlying experiment was conducted by generating, for fixed N , several hundred RCMs of Gram type, $C = TT^*$, with T an $N \times (N+1)$ matrix with row vectors distributed

<p style="text-align: center;">TABLE 2-1</p> <p style="text-align: center;">Correlation Matrices with Indefinite</p> <p style="text-align: center;">Toeplitz Projections</p>			
	C	C_T	min σ (C_T)
N = 4	1.0 .697 -.709 -.911 1.0 -.747 -.702 1.0 .611 1.0	1.0 .187 -.705 -.911	-.117
N = 5	1.0 .252 -.168 -.493 -.904 1.0 -.614 .583 -.239 1.0 -.613 -.203 1.0 .353 1.0	1.0 -.155 .206 -.366 -.904	-.144

independently and uniformly over the sphere S^N in R^{N+1} . The resulting matrices were then projected onto T_N and their eigenvalues computed via IMSL routine EIGRS, an eigen-program designed for real symmetric matrices.

These findings seem rather curious and deserving of further study. We note that the set $\Gamma(N)$ of real $N \times N$ correlation matrices is a compact convex set of dimension $N(N-1)/2$. The fact that this is rapidly increasing with N suggests that perhaps we do not have a sufficiently large sample size for $N \geq 16$ in Table 2-2 to be able to conclude much about the ‘true’ probability that an $N \times N$ RCM has a Toeplitz correlation matrix as its projection. But the fact that these projections can occasionally fail to be positive definite means that the following simple algorithm for generating TRCMs cannot be guaranteed failproof:

- Generate a RCM C ;
- Return C_T .

For this reason it cannot be recommended for numerical work.

Method 5 As discussed at some length in [11], one natural criterion for a class of RCMs to be ‘truly random’ is that the associated class of spectra be uniformly distributed over the simplex $S_N = \{\lambda_i \geq 0 : \sum \lambda_i = N\}$ of appropriate dimension. We will discuss some tests of such randomness for the TRCMs produced by Methods 2 and 3 in the next section. But first we want to take note of a recently proposed algorithm which might permit a direct solution of the problem of generating TRCMs with random spectrum.

<p style="text-align: center;">TABLE 2-2</p> <p style="text-align: center;">Empirical Failure Rate of RCM to</p> <p style="text-align: center;">Project onto TRCM</p>			
	No. Trials	No. Failures	Failure Rate
N = 3	500	0	.000
4	500	11	.022
5	500	8	.016
8	500	5	.010
16	500	0	.000
24	300	0	.000
32	200	0	.000

Since it is easy to sample randomly (i.e., uniformly) from the simplex S_N , the issue quickly reduces to the possibility of constructing a Toeplitz correlation matrix with a given spectrum. In general (for $N \geq 5$) it is unknown if this problem always has a solution; this is the ‘inverse Toeplitz eigenproblem.’ Nevertheless, a recent article by D. Laurie [13] offers a numerical procedure which, in spite of the lack of a convergence proof, is claimed to solve this problem in practice, in fact, to exhibit quadratic convergence.

Let $\{\lambda_i\} \subset \underline{R}$ be a tentative spectrum of a real symmetric Toeplitz matrix, and set $\Lambda = \text{diag}[\lambda_1, \dots, \lambda_N]$. If T is such a matrix then there must be an orthogonal matrix Q such that $T = Q\Lambda Q^*$ or, equivalently, $Q^*TQ = \Lambda$, a diagonal matrix. Laurie’s algorithm involves a succession of alternate orthogonal diagonalizations of a symmetric Toeplitz matrix, followed by a new choice of Toeplitz matrix so that its diagonal, under the current orthogonal basis, agrees with Λ . This latter step amounts to solving an $N \times N$ linear system, arising from use of the basis vectors for the subspace T_N discussed earlier under Method 4. Some simplifications are possible due to the reciprocal structure of the eigenvectors of a Toeplitz matrix. Various Toeplitz starting values are suggested.

In spite of the alleged rapid convergence properties of this procedure, it still seems like a lot of work to undertake to obtain TRCMs, with a fair potential for round-off accumulation. For this reason we have not attempted to program and operate this method. We have included it in this discussion because it does present, granting convergence and round-off control, a method for producing TRCMs with random spectrum. We remark that the inverse Toeplitz eigenproblem has been raised in an earlier RCM context by Marsaglia and Olkin [15].

3. NUMERICAL EXPERIENCE

In this section we summarize some computer experiments with Methods 2, 3, and 4 of the previous section. There is clearly any number of questions that one can raise concerning the distribution of various spectral functions of TRCMs for a specific probabilistic generating mechanism. However, the study of such questions was never our goal for undertaking this work. Rather, as discussed in the introductory section, we are primarily interested in a fast and reliable method for generating TRCMs with a nicely dispersed spectrum, that is, TRCMs whose spectrum is more or less uniformly distributed over the simplex S_N .

At the end of the previous section we noted that Laurie's algorithm when combined with a generator for sampling from the uniform distribution over S_N provides the most direct conceptual solution of this problem, yet appears not to be 'fast,' relative to the other methods. So what we really want to see now is whether some of the other, faster, methods can be said to yield TRCMs with a random spectrum.

How might we try to decide, absent a definitive theorem, whether a given class of TRCMs has a random spectrum? This is a matter that was discussed at some length in our earlier report [11]; however, the central issues will be briefly recalled next.

First, we say that an $N \times N$ random correlation matrix A has a random spectrum if its spectrum $\sigma(A)$, viewed as a point in the simplex S_N , is uniformly distributed over S_N . Now, one way to obtain this distribution is by means of the spacings determined by a sample from the standard uniform distribution on the interval $[0, 1]$. Namely, if $u_{(1)} \leq \dots \leq u_{(N-1)}$ are the order statistics of a random sample drawn from $U[0, 1]$, and we put $u_{(0)} = 0, u_{(N)} = 1$, then the *spacings* of this sample are defined by

$$s_i = u_{(i)} - u_{(i-1)}, \quad i \leq i \leq N.$$

The spacings are positive numbers (with probability one), and sum to unity. As noted in [11], it can be proved that the vector $N(s_1, \dots, s_N)$ is uniformly distributed over S_N .

Now suppose given, for some fixed N , a sample of size n of $N \times N$ TRCMs generated by some particular procedure; for example, by Method 2 or 3. For each matrix C in the sample we compute its spectrum $\sigma(C)$. There are now (at least) two general types of tests that can be applied to test the null hypothesis that $\sigma(C)$ is uniformly distributed over S_N . The first type consists of computing a functional $f(\sigma(C))$ of the spectrum whose distribution, under the null hypothesis, is known. The second type involves a transformation $T : S_N \rightarrow [0, 1]$; we evaluate $T(\sigma(C))$ obtaining a finite subset of $[0, 1]$ and test that this sample is from $U[0, 1]$. (Transformations of S_N onto other simplicial regions, and tests against uniformity there are also possible; one such transformation is simply projection on the first $N - 1$ coordinates.)

Examples of the first type of test are given by choosing the spectral functions f as

$$\begin{aligned} f(\lambda_1, \dots, \lambda_N) &= \max(\lambda_i), \text{ or} \\ &= \min(\lambda_i), \text{ or} \\ &= \sqrt{(\lambda_1^2 + \dots + \lambda_N^2)}. \end{aligned} \tag{3.1}$$

These functions are, respectively, $\|C\|$, $\|C^{-1}\|$, and $\|C\|_F$ (the Frobenius norm of the matrix C). An example of the second type of test is given by choosing the transformation T as $T(\lambda_1, \dots, \lambda_N) = (x_1, \dots, x_{N-1})$, where

$$\begin{aligned} x_1 &= \lambda_1/N, \\ x_2 &= x_1 + \lambda_2/N, \\ &\dots\dots\dots \\ x_{N-1} &= x_{N-2} + \lambda_{(N-1)}/N. \end{aligned} \tag{3.2}$$

We see that $0 < x_1 < x_2 < \dots < x_{N-1} < 1$, and that the associated spacings are given by $s_k = \lambda_k/N$, $1 \leq k \leq N$.

Under the null hypothesis H_0 of a random (uniform) spectrum, each of the random variables defined by Equation (3.1) has a distribution about which much is known; see the discussion in [11, Sec. 4]. In particular, the distribution of $\|C^{-1}\|$ is available in closed form:

$$Pr(\|C^{-1}\| > x) = (1 - x)^{N-1}, \quad 0 < x < 1, \quad (3.3)$$

while the other two distributions have closed-form asymptotic expressions.

If, on the other hand, we elect to utilize the transformation $T : (\lambda) \rightarrow (x)$ defined by Equation (3.2), then we will arrive at n samples (x) which, under the null hypothesis, are each drawn from $U[0, 1]$. Each of these may then be subjected to a goodness-of-fit test for uniformity, of which there are many. Some fraction of these will presumably pass such a test, and we will then have to decide whether this fraction is large enough so as not to reject H_0 .

A third alternative is to view each sample (x) as a single point in the cube $[0, 1]^{N-1}$. Under H_0 this set of n points is a random sample from $U[0, 1]^{N-1}$, and a multivariate goodness-of-fit test for uniformity could be applied. This approach is really more definitive than the one just discussed but, especially for large N , would require much larger sample sizes than what are presently available.

How are we to choose among this multitude of plausible tests? Classical statistical theory suggests that we consider power. But this too is a multi-layered task. Variables here include, besides the different tests, sample size and alternative hypotheses. That is, different tests will exhibit different powers against different types of alternatives, and as the sample size varies. It is certainly not our intent here to engage in a serious study and ranking of the many possible tests for uniformity of spectrum. Rather we shall just report, as a rough guide, results from two such tests in the case of Methods 2 and 3.

We first consider the test based on the least eigenvalue which, under the null hypothesis of uniform spectrum, has the distribution given by Equation (3.3). From each of the two methods for generating TRCMs, we obtain a sample of size $n = 100$, for $N = 5, 10$, and 20 , compute the spectrum, and then the empirical distribution function of the least eigenvalue. This is then compared with the theoretical distribution in a Kolmogorov Smirnov one-sample test.

In the case of TRCMs generated by Method 2, this test decisively rejected uniformity of spectrum. The K-S test statistic is highly significant, as shown by the values on the top line of Table 3-1. The problem is that the least eigenvalue is too large, as can be seen in the case $N = 10$ from Figure 3-1. It displays the empirical and theoretical distributions, and also indicates that the average least eigenvalue = 0.2596, with a sample standard deviation of 0.1383. Under the null hypothesis, the expected value of the least eigenvalue is $1/N = 0.1$, here, with variance = $(N - 1)/N^2(N + 1) = 0.00818$, here. Hence the sample average should be approximately $N(0.1, 0.0000818)$ distributed, which is clearly incompatible with the data.

TABLE 3-1 K-S Test Statistics for Minimum Eigenvalue of TRCM			
	N = 5	N = 10	N = 20
Method 2	5.42	5.54	7.75
Method 3	1.91	1.96	2.05

The case of TRCMs generated by Method 3 is more ambiguous, partly because of the choice of the parameters L and σ . Certainly there are ‘bad’ choices of these parameters. We have only mildly tried to optimize this choice: the data reported in the lower half of Table 3-1 is based on the case $L = 3N$ and $\sigma = 7N$. We see that the K-S statistic is still significant (values > 1.63 are significant at the 1% level). But the sample mean is only about 2σ away from its mean under the null hypothesis. Overall, this case presents a much less emphatic rejection of uniformity that associated with Method 2. See Figure 3-2 for comparison.

Our second test involves the use of Neyman’s statistic N_2 . The theory of this test is available in several sources, for example [19]. In general, there is a sequence $\{N_k : k = 1, 2, \dots\}$ of statistics

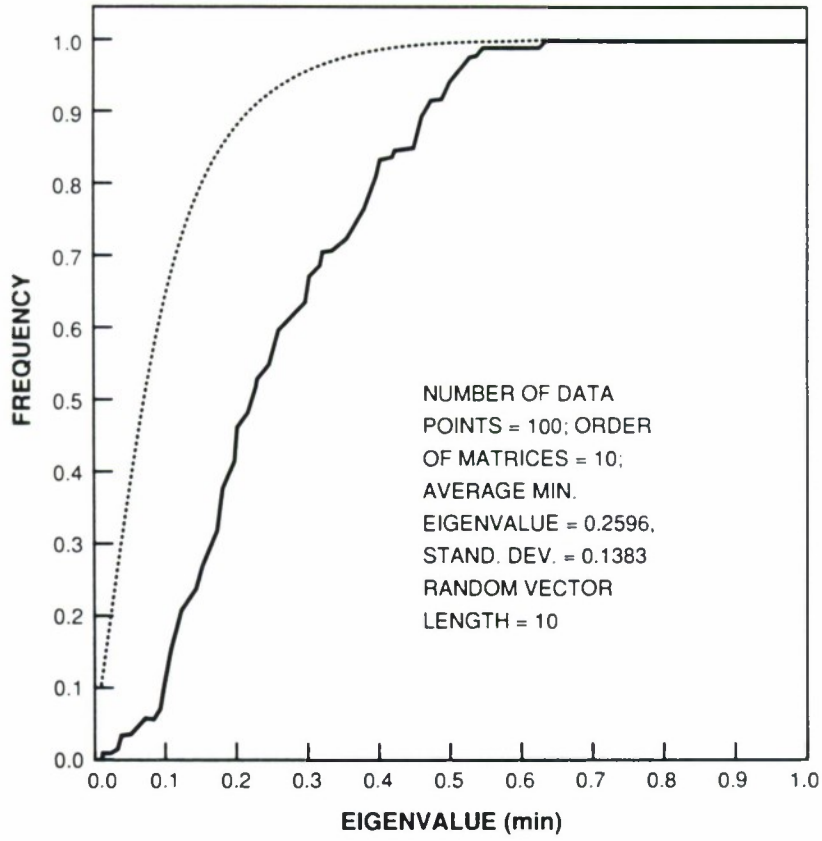


Figure 3-1. Frequency distribution of minimum eigenvalues: Random Toeplitz Method 2.

that can be used to test the hypothesis of uniformity on $[0, 1]$ against an alternative density of the form

$$f(x) = c \exp \left\{ 1 + \sum_{j=1}^k b_j l_j(x) \right\},$$

where the l_j are Legendre polynomials, and c is a normalizing constant whose precise value depends on $\{b_j\}$. The null hypothesis is $H_0 : b_j = 0$, for all j , or, equivalently,

$$H_0 : \sum_{j=1}^k b_j^2 = 0.$$

The Neyman statistic $N_k = v_1^2 + \dots + v_k^2$, where

$$v_j = \sqrt{\frac{1}{n}} \sum_{i=1}^n l_j(x_i),$$

and $(x_i : i = 1, \dots, n)$ is the sample. It follows that when $k = 2$, N_2 is a combination of the sample mean and variance and thus has an intuitive appeal. It is known that each N_k is asymptotically distributed as $\chi^2(k)$, and that tests based on N_k , which result in rejection of the null hypothesis for large values of N_k , are consistent and asymptotically unbiased. In practice, the $\chi^2(s)$ approximation to N_2 is quite accurate for $n \geq 20$; for small n , upper tail percentage point tables are available.

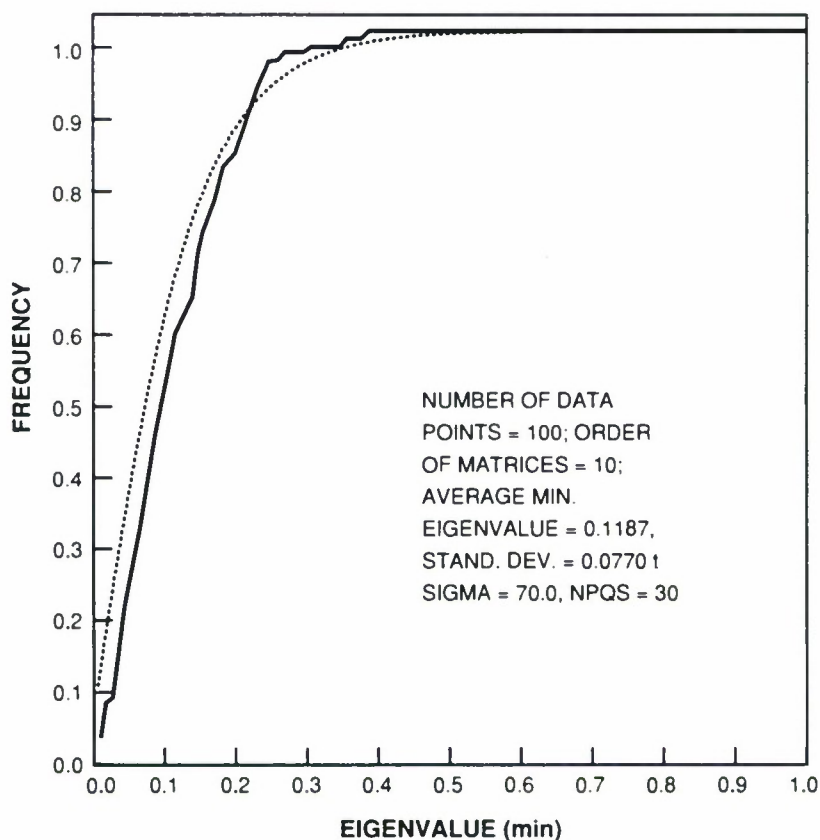


Figure 3-2. Frequency distribution of minimum eigenvalues: Random Toeplitz Method 3.

We computed the Neyman statistics N_2 for the same batches of TRCMs as were tested using the least eigenvalue statistic. The results are summarized in Table 3-2 below. For each of Methods 2 and 3, and each dimension $N = 5, 10$, and 20 , we give the average and standard deviation of the 100 N_2 's computed from each TRCM, and also the empirical percentage of the sample whose N_2 - value exceeded the .01 significance level. This level, for the cases $N = 5, 10$, and 20 is, respectively, 9.64, 9.26, and 9.23.

The main inference to be drawn from this data is that as the matrix size N increases beyond 10 , we observe ever more pronounced deviations from uniformity, so we would have to reject the hypothesis of uniformity for TRCMs generated by either of these methods for $N > 10$.

TABLE 3-2				
Neyman N2 Statistic Summary for TRCM				
Method 2		N = 5	N = 10	N = 20
	Ave.	1.62	4.16	9.10
	S.D.	0.86	1.94	3.30
	Sig. 0.01	0%	3%	39%
Method 3		N = 5	N = 10	N = 20
	Ave.	2.62	5.53	11.50
	S.D.	0.99	1.69	2.52
	Sig. 0.01	0%	3%	83%

Our conclusion, based on both tests, is that for $N \leq 10$, Method 3, with proper choice of its parameters L and σ , can be said to produce TRCMs with uniform spectrum. It may be possible, for larger N , to adjust these parameters in Method 3, so as to pass these tests for uniform spectrum. Failing that, and insofar as a random spectrum is deemed desirable, we must fall back on the as yet untried Method 5.

4. LOOSE ENDS AND OPEN QUESTIONS

In this final section we collect together a number of remarks pertinent to the foregoing material, and unresolved issues that appear worthy of further study. These latter issues are certainly of varying degrees of difficulty, running as they do from further simulation work to rather deep theoretical issues.

4.1 Approximation of Toeplitz Correlation Matrices

Given that our primary interest in TRCMs is that they serve as the covariance matrices of sections of stationary stochastic processes, it is conceivable that simple models for such processes might yield an adequate supply of TRCMs. Of course, the terms ‘simple’ and ‘adequate’ must be carefully specified.

Let us say that ‘simple’ means an autoregressive process of some order m , which we denote by $AR(m)$. The cases $m \leq 2$ are of particular interest. When $m = 1$, the corresponding $N \times N$ correlation matrices C_ρ are indexed by the real parameter ρ , $|\rho| \leq 1$, and the eigenvalues of C_ρ are known [17] to be of the form

$$\lambda_k = \frac{1 - \rho^2}{1 - 2\rho \cos \omega_k + \rho^2}, \quad 1 \leq k \leq N,$$

where the ω_k must be obtained numerically from a nonlinear equation. When $m = 2$, the eigenvalues are not similarly available in closed form, but can still be indexed by a pair of real parameters. For instance, correlation matrices of the form given by Equation (2.4), with

$$\phi(t) = \exp(-\alpha |t|) \cos 2\pi\beta t,$$

can occur. (In $m = 1$ case, the cosine term would be absent.)

By ‘adequate’ we might mean either the degree of density or coverage of the class of all $N \times N$ Toeplitz correlation matrices by those corresponding to the $AR(m)$ processes, or the degree of coverage of the eigenvalue simplex S_N by the spectra of these matrices. Can either of these degrees of coverage by correlation matrices of $AR(m)$ be quantified as a function of m ? And if so, is it small enough to permit usage of these special matrices for the intended applications? But the real problem may be that, even if the previous questions can be answered affirmatively for some $m < N$, it will prove to be overly difficult to actually generate the correlation matrices corresponding to the appropriate $AR(m)$ processes, relative to the methods of Section 3.

We remark that rational approximation in the frequency domain may be a plausible approach to the first question above.

4.2 Length of Random Vector in Method 2

In this method the key step was a random draw from the unit sphere in \underline{R}^N . It is possible to draw instead from the unit sphere in a larger space \underline{R}^L , $L > N$, and still define the function ϕ as

before. One might ask how the spectral properties, in particular the spectral distribution of the resulting TRCM, depend on this parameter L . A brief look at this problem has suggested that the distribution of eigenvalues does not become more uniform, contrary to both hope and expectation.

4.3 Random Probability Distributions

This probably is the most interesting theoretical concept to arise in the present study. In the context of Method 3 we have discussed one possible approach to this problem, namely, the use of the Dirichlet process. We noted that conventional methods as well as our *ad hoc* approach yielded discrete probability measures. Here we want to mention another, more recent, procedure for selecting a probability measure on \underline{R} at random that, with probability one, yields absolutely continuous measures with an analytic density. So, in a sense, we are at the opposite extreme from the Dirichlet distributions.

This procedure is due to Chen and Rubin [4, 5], and is based on the use of an orthonormal basis for $L^2(\underline{R})$. (Other measure spaces besides $(\underline{R}, \text{Leb.})$ could be used, but as these are taken more abstract, some of the special properties known for the resulting densities, such as analyticity, existence of moments, etc. may be lost.) If $\{\phi_n\}$ is such a basis, and $b = \{b_n\}$ a sequence of scalars such that $\sum b_n^2 = 1$ (notation: $b \in S(l^2)$), then the function:

$$f(x) = \left| \sum_n b_n \phi_n(x) \right|^2 \quad (4.1)$$

is easily seen to be a probability density function (pdf) on \underline{R} . It follows that any procedure for selecting sequences b randomly from the sphere $S(l^2)$ will lead to a random pdf via Equation (4.1).

Of course there is a difficulty here in that the Hilbert space l^2 is of infinite dimension and hence its spheres are noncompact. Further, there is no rotationally invariant probability measure on $S(l^2)$, although there are finitely additive measures on the algebra of cylinder sets of l^2 which are rotationally invariant, for instance, the canonical Gauss measure. But in order that a cylinder set measure can be extended to be a countable additive measure on a Borel set of l^2 , its covariance operator must be nuclear [1]. This means that its spectrum is composed of eigenvalues converging rapidly enough to zero so as to form a summable sequence. Hence the associated measure is highly anisotropic.

Actually, there is a second difficulty here besides the conceptual one associated with the idea of a uniform distribution on the sphere $S(l^2)$, and that concerns the necessity to approximate infinite dimensional vectors by finite dimensional ones. That is, in practice the sum in Equation (4.1) must be truncated. Fortunately, sums of generally not unreasonable length suffice to approximate ‘most’ pdfs, as shown in [4]. There remains the task of numerical simulation of random draws from $S(l^2)$ to achieve such approximations. One scheme suggested in [4] yields an expected dimension of about 50. One can imagine also other schemes for doing the simulations.

The point to be made here is that we have here a new method for producing random pdfs which in turn will lead via Method 3 to TRCMs, and we do not have any information at this time

as to how the spectral properties of these matrices behave. Note, however, a practical drawback to the use of these densities for generating TRCMs in that much more computational effort must be expended in order to compute their Fourier transforms, in comparison with the case of discrete probability measures.

A final comment is to recall that orthonormal series have been long used as one of several popular approaches to nonparametric probability density estimation. That is, an estimate of an unknown pdf f is constructed by using a given sample to form estimates of a finite number of Fourier coefficients of f with respect to the given basis. This method dates from work of N. Chencov, 1962, with further contributions by S. Schwartz, G. Watson, R. Kronmal and M. Tarter, and D. Bosq, *inter alia*. Possibly familiarity with this approach to density estimation served as some motivation for the Chen-Rubin approach to density construction. We note that while their densities are nonnegative by definition, as they should be, the conventional pdf estimators can well lack this property (particularly for small data samples), a well-known shortcoming of the orthogonal series method.

4.4 Other Issues in Method 3

There are several parameters that can be varied: the integer L (number of point masses), the variance parameter σ (spread of the points about the origin), and the points $\{t_i\}$ themselves. We have used $t_j = j$ in Equation (2.5), but other choices are possible, and might lead to improved (more uniform) spectral distributions. Also, the set $\{t_j\}$ might be randomized.

There seems to be a distinct lack of theoretical results about these specific questions, although there is certainly no lack of theory of symmetric Toeplitz matrices. We have in mind especially results about the asymptotic behavior of eigenvalues. Such theorems might help shed light on the spectral behavior of large TRCMs generated by either of Methods 2 or 3.

If the urn scheme of Equation (2.7) is used to build up discrete Dirichlet-distributed probability measures, how do the resulting TRCMs behave?

4.5 Effect of the Toeplitz Projection

Recall that the projection operation $C \rightarrow C_T$ described in Method 4 could not be guaranteed to ‘work,’ in the sense of always returning a (Toeplitz) correlation matrix C_T whenever a correlation matrix C was input. Nevertheless it ‘usually’ works. This phenomenon seems worthy of further understanding and quantification. Is it possible to assign a probability to the statement ‘ $C_T \in \Gamma(N)$ if $C \in \Gamma(N)$ ’?

More generally, one might inquire if there are any general facts about changes in spectrum induced by projections in the space of square matrices with the Hilbert-Schmidt inner product of Equation (2.8). A particular question is what the Toeplitz projection does to a class of RCMs with uniform spectrum, at least in those cases where it preserves the positivity.

Apropos of this last question, there arises a certain practical matter: how does one produce a sequence of RCMs with a uniform spectrum? Note that this is not a theoretical difficulty — one begins with any positive definite matrix with a desired spectrum in S_N and then sequentially adjusts the diagonal entries via a sequence of Givens rotations. This method is discussed in [11], with alternate references provided, and it is noted that the IMSL subroutine GGCOR provides a commercial package for this very purpose (this subroutine will also make random draws from the orthogonal group $O(N)$). The problem is that, as the subroutine documentation warns, the spectrum of the final matrix may differ from the initial input spectrum. In fact, this problem seems to be very real. In 100 trials each for $N = 3, 5, 8$, with an initial spectrum drawn randomly from the uniform distribution $U(S_N)$, we observed an empirical failure rate of 0.3% (resp., 7%, 18%). That is, these percentages of the trials resulted in nonpositive definite output matrices.

4.6 Toeplitz RCMs with Random Spectrum

We have seen that, especially for matrices of order $N > 10$, we do not have as yet a method of producing Toeplitz RCMs with a random (uniform) spectrum other than Method 5, with which we have no direct experience. We have mentioned the basic questions of existence and convergence associated with this method, and the probable difficulties with implementation and round-off.

Another basic question which needs to be recorded in this context is whether we should expect the existence of TRCMs with random spectrum. Our numerical work leads us to accept this hypothesis for small orders ($N \leq 10$), but is otherwise inconclusive. But, in any event, there is no existence theorem, and the connection between such a result, if true, and the inverse eigenvalue problem for Toeplitz correlation matrices should be explored. Certainly, if the inverse eigenvalue problem is solvable, and the convergence of Method 5, or some other, is validated, then we will have a source of TRCMs with random spectrum. And, in the converse direction, if TRCMs with random spectrum, can be constructed, then, with arbitrarily high probability, we can find a Toeplitz correlation matrix with a given spectrum. (Sketch of argument ... Let $0 < p_n \uparrow 1$, and V_n be a decreasing sequence of open sets in the simplex S_N with $\cap V_n = \{\lambda_0\}$. Then with probability $> p_n$ there is a Toeplitz correlation matrix T_n with $\sigma(T_n) \in V_n$. By compactness of the set of $N \times N$ correlation matrices, there is a convergent subsequence of $\{T_n\}$ with limit T , and by standard results on spectral perturbations, $\sigma(T) = \{\lambda_0\}$. The probability that the first m of the T_n exists is $p_1 \dots p_m$ and, if the increase of p_n to 1 is sufficiently rapid, this partial product will coverage to a number arbitrarily close to 1.)

4.7 Further Simulation and Power Studies

Failing theoretical advances, there is always the possibility of further numerical work along the lines reported in Section 3. This might take the form of either additional tests for uniformity or, more interestingly, studies comparing the power of various tests for uniformity relative to a particular alternative. In particular, is there a uniformly most powerful test for uniformity?

As an example we looked at a statistic of Lohrding [14] which was shown to have favorable power against various alternatives with respect to other popular test statistics such as Kolmogorov-Smirnov and Cramer-von Mises. In the case where we are testing an ordered sample $\{x_1, \dots, x_{N-1}\}$ for uniformity on $[0, 1]$, the test statistic in question is

$$T = (d_1 + \dots + d_{N-1})/(N - 1),$$

where

$$d_k = |x_k - m_k|/c_k;$$

here m_k and c_k^2 are the mean and variance of the k th order statistic from a sample of size $N - 1$ from $U[0, 1]$. Use of this statistic for TRCMs generated from Methods 2 and 3 basically reconfirmed results reported in Section 3 for the other two tests, by leading to rejection of the null hypothesis for $N > 10$.

5. SUMMARY

The theory and practice of random Toeplitz correlation matrices is more subtle than that of random correlation matrices. This is to be expected given the corresponding greater mathematical difficulties with Toeplitz matrices and operators vis-a-vis Hermitian matrices and operators. Starting from this background, we prepared this report with two goals in mind: to raise several theoretical issues concerning the spectral behavior of Toeplitz RCMs, and to present some numerical experience with certain special cases.

In fact, a variety of unresolved theoretical questions arose in the course of this work, and these are collected together in Section 4. The most interesting of these appear to be (1) the spectral behavior of Toeplitz RCMs generated from the characteristic functions of various random probability measures; (2) the connection between the inverse eigenvalue problem for Toeplitz correlation matrices and the concept of Toeplitz RCMs with random (uniform) spectrum; and (3) the behavior of the matrix spectrum under the Toeplitz projection operator.

The numerical results shed varying degrees of light on some of the theoretical questions, as we have tried to indicate. Insofar as the matter of computer generation of Toeplitz RCMs is concerned, we are left with Method 3 (based on the characteristic functions of random discrete probability measures) as the method of choice. This method is not quite as efficient as Method 2 (based on the autocorrelation function of a random discrete moving average process), but seems to yield more uniformly distributed spectra. But the tests of both methods for uniformity fail for moderately large matrix sizes ($N > 10$), and so that area remains open too.

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