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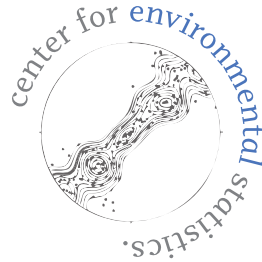
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A HORSESHOE FOR MULTIDIMENSIONAL SCALING

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ABSTRACT. Horseshoes (quadratic curves) routinely show up in multidimensional scaling and correspondence analysis solutions. We review some of the empirical situations in which they are known to occur, and we discuss some of the mathematical models that produce them. One particular model, discussed by Diaconis et al. in a recent paper, is the Kac-Murdock-Szegö matrix A with elements $a_{ij} = \rho^{|i-j|}$. In this paper we analyze this example in some detail. We point out that A is both totally positive and Toeplitz, and that the horseshoes also occur for other matrices with these properties. It is shown that double centering of a Toeplitz matrix leads to a centro-symmetric matrix, which again will produce horseshoes.

1. INTRODUCTION

Horseshoes and similar structures have been observed in many MDS examples, and in related data analysis techniques such as Principal Component Analysis (PCA), Correspondence Analysis (CA), and Multiple Correspondence Analysis (MCA) as well. Empirical examples in MDS include the classical Ekman color circle and the Plomp-Levelt parabolic musical intervals [Shepard, 1974]. One can argue that the parametric mapping techniques in Shepard and Carroll [1966] were intended to unfold these classical horseshoes.

In political science the horseshoe, curving from left (progressive) to right (conservative), has been observed in many countries. A good example is De Gruijter [1967], where the horseshoe folds further into an ellipse on which the two extremes meet. In De Leeuw and Mair [submitted] an MCA analysis is presented of roll-call votes in the US senate, where the three-dimensional dimensional solution consists of two disjoint horseshoes, one for democrats and one for republicans.

Hill [1974], in one of the earliest articles on CA in English, notes that horseshoes are commonly found in the analysis of ecological and archeological incidence and abundance matrices. He propose Detrended Correspondence Analysis to unfold the horseshoes into linear dimensions, because he considers them to be mathematical artifacts, without empirical content, that moreover waste a dimension by presenting one-dimensional structures in the plane. Further examples can be found in archeology, where Kendall [1971] used MDS in his HORSHU method of seriation.

Mathematical conditions leading to horseshoes have been studied in the various disciplines that encounter them. In Guttman [1950] it was shown that a CA of the perfect scale leads to curvilinear dimensions, because the eigenvectors satisfy the three-point recursions defining the classical orthogonal polynomials, also familiar from discrete Sturm-Liouville boundary value problems. Further work along these lines is in Iwatsubo [1984]. Work of Lancaster [1969], and his many co-workers, has shown how horseshoes, in the form of orthogonal polynomials, show up in the CA of many bivariate distributions. In CA the horseshoe is so common

that the Analyse des Données school of Benzécri describes it in detail as the "Effect Guttman". See, for example, Benzécri [1980, Ensemble VII].

More generally, in Schriever [1983, 1985] the Gantmacher-Krein-Karlin theory of total positivity was used to give general conditions for horseshoes that show up in the form of oscillating and interlocking eigenvectors. It was shown by Schriever, and also by Gifi [1990, Chapter 9], that many of the popular latent trait models lead to horseshoes. In ecology, for example, the Gaussian Ordination Model for abundance data gives horseshoes in CA. In archeology unimodal frequency matrices or Q-matrices have the same effect. In a recent chapter De Leeuw [2008] reviews much of the archeological and ecological literature on horseshoe effects.

2. Problem

In Diaconis et al. [submitted] a symmetric matrix of order n

$$D^{(2)} = e_n e_n' - A,$$

is defined, where e_n is a vector with all n elements equal to one, and where A has elements $a_{ij} = \exp(-\sigma|i-j|)$, with $\sigma > 0$ some positive number. Classical Multidimensional Scaling (MDS) [Torgerson, 1958] is applied to $D^{(2)}$, pretending it is a matrix of squared Euclidean distances. Let J_n be the centering matrix, i.e. $J_n = I - \frac{1}{n} e_n e_n'$. Define $\tilde{A} = J_n A J_n$. Classical MDS computes the eigenvalues and eigenvectors of $\tilde{A}$.

Diaconis et al. [submitted] use this example to show how MDS can lead to horseshoes. Their main empirical example comes from political science roll-call data. Their technique imbeds the discrete problem into a related one with continuous kernel. The eigenvalue problem for the continuous kernel is solved, and perturbation techniques are used to derive approximate results for the original discrete data structure.

Note that if we define $\rho = \exp(-\sigma)$, then $0 < \rho < 1$, and we can write A in the simpler form $a_{ij} = \rho^{|i-j|}$. Note that it sometimes makes sense to write $A(\rho)$ to indicate the dependence on ρ, and some time even to write $A_n(\rho)$ to indicate that we are dealing with the leading principal submatrix of order n of the infinite matrix $A_\infty(\rho)$.

The matrix A is the autocorrelation matrix of a stationary AR(1) process, and it has been studied extensively in Kac et al. [1953], see also Grenander and Szegö [1958]. All our key results are essentially given in those references, and in computational form they are already in Trench [1988], where A is called the Kac-Murdock-Szegö matrix. We will also use this name, and abbreviate it to KMS-matrix. Thus there is nothing in this note that is not at least 50 years old, except perhaps the way in which we introduce the results. We do not use continuous kernels, and we introduce increasing structure by using more and more properties of the matrix A.

Note that we derive most of results for A, although MDS analyzes $\tilde{A}$. But a detailed study of A is necessary before we get to the results for $\tilde{A}$ in the final section.

3. On KMS Matrices

We start with two simple and general properties of A that are immediately obvious.

Result 1. A is a correlation matrix with positive elements. Thus, by the Perron-Frobenius Theorem, it has a simple largest eigenvalue, corresponding with an eigenvector with positive elements.

Proof. The Perron-Frobenius Theorem is, for example, in Gantmacher and Krein [2002, p. 83]. □

Result 2. A is positive definite. Thus all its eigenvalues are positive.

Proof. This follows from the interpretation of A as the autocorrelation matrix of an AR(1) sequence. □

3.1. **A is Totally Positive.** We now use more structure, and show that A is totally positive (TP), i.e. all its minors of any order are positive. The two classical references on total positivity are Gantmacher and Krein [2002] and Karlin [1968]. Note that the first Russian edition of the Gantmacher-Krein book is from 1941, the first English translation was published in 1950.

Result 3. A is a single-pair matrix, also known as a Green's matrix [Karlin, 1968, p. 110-112], and is consequently TP.

Proof. See Gantmacher and Krein [2002, p. 78]. Let $\psi_i = \rho^{-i}$ and $\chi_i = \psi_i^{-1} = \rho^i$. Then

$$
a_{ij} = \begin{cases} \psi_i \chi_j & (i \leq j), \\ \psi_j \chi_i & (i \geq j). \end{cases}
$$

Since all ψ_i and χ_i have the same sign, and since

$$
\frac{\psi_i}{\chi_i} = \rho^{-2i}
$$

strictly increases, the conditions of Gantmacher and Krein [2002, p. 79, result (c)] are satisfied. In fact, below their result (c), Gantmacher and Krein explicitly mention our A, which they write as G_σ. □

Result 4. The inverse of A is a symmetric tri-diagonal matrix.

Proof. See Gantmacher and Krein [2002, p. 82, result (g)] for the tri-diagonal form of the inverse. □

Result 5. The eigenvalues of A satisfy $\lambda_1 > \lambda_2 > \cdots \lambda_n > 0$.

Proof. See Gantmacher and Krein [2002, p. 87, Theorem 6]. □

The most interesting aspect of total positivity is that we can already see where the horseshoes come from, even though we are using relatively few properties of A. Those properties A has in common with the very large number of examples mentioned by Karlin and Gantmacher and Krein that are also TP, and that will consequently also lead to horseshoes. This was first explored systematically in a multivariate data analysis context by Schriever [1983, 1985].

We need some additional notation. Suppose x_k is the eigenvector of A corresponding with eigenvalue λ_k, the kth largest eigenvalue. We can plot the n elements of x_k against $1, 2, \cdots, n$ and connect successive points. The zero-crossings of the resulting piecewise linear function are called the *nodes* of the eigenvector.

Result 6. Eigenvector u_k has exactly $k - 1$ sign changes. The nodes of successive eigenvectors interlace, i.e. the $k - 1$ nodes of x_k separate the k nodes of x_{k+1}.

Proof. See Gantmacher and Krein [2002, p. 87, Theorem 6]. They actually give a stronger result on sign changes of linear combinations of eigenvectors.   □

It is shown by Schriever [1985, p. 48-55] that total positivity is already sufficient for the CA of the matrix to give a horseshoe, in the sense of a convex or concave curve, if we plot the n elements of the first and second eigenvector in the plane, and connect successive points. Actually the weaker condition TP(2), which only assumes that all minors or orders one and two are positive, is already sufficient.

Remark 1. It may be of interest that $a_{ij} = \exp(-(x_i - x_j)^2)$ is TP for all x. In this case we do not need equal spacing. This example is relevant for the Gaussian Ordination Model in ecology [Ter Braak, 1985].

3.2. **A is Toeplitz.** From the fact that A is TP we know that there are no muliple eigenvalues, that the kth eigenvectors has $k - 1$ sign changes, and that the eigenvectors have interlacing nodes. We can get some interesting symmetry properties for the eigenvectors by using the fact that A is Toeplitz. Remember that a symmetric matrix A is Toeplitz if there are numbers $t_0, t_1, \cdots, t_{n-1}$ such that $a_{ij} = t_{|i-j|}$.

Result 7. A is a symmetric Toeplitz matrix with $t_i = \rho^i$.

Suppose K_n is the matrix of order n with ones on the secondary diagonal and zeroes everywhere else. We say that a vector x is symmetric if $K_n x = x$ and skew-symmetric if $K_n x = -x$. We will say that eigenvalues of A corresponding with symmetric eigenvectors form the *even spectrum*, while those corresponding with skew-symmetric eigenvalues form the *odd spectrum*.

Result 8. A has $\lceil \frac{n}{2} \rceil$ symmetric and $\lfloor \frac{n}{2} \rfloor$ skew-symmetric eigenvectors.

Proof. This result is usually attributed to Cantoni and Butler [1976]. Because A is Toeplitz we have $K_n A K_n = A$. Also $K_n^2 = I$, which means all

eigenvalues of K_n are ± 1. Thus if $Ax = \lambda x$, then $K_n A K_n x = \lambda x$, and $A K_n x = \lambda K_n x$. If λ is simple we must have $K_n x = \mu x$ for some μ, and thus $K_n x = \pm x$. This shows eigenvectors of A are either symmetric or anti-symmetric.

We can go one step further, following the notation of Delsarte and Genin [1983], by defining

$$(1) \qquad M_n = \frac{1}{\sqrt{2}} \begin{bmatrix} I_p & I_p \\ K_p & -K_p \end{bmatrix}$$

Here we assume n is even and the matrices I_p and K_p are of order $p = \frac{n}{2}$. Now $M'M = MM' = I$. A Toeplitz matrix (of even order) can be written in the form

$$A = \begin{bmatrix} A_1 & A_2 K_p \\ K_p A_2 & A_1 \end{bmatrix}$$

with both A_1 and A_2 symmetric of order p. Now

$$M'AM = \begin{bmatrix} A_1 + A_2 & 0 \\ 0 & A_1 - A_2 \end{bmatrix},$$

or $M'AM = (A_1 + A_2) \oplus (A_1 - A_2)$. Thus the eigenvectors of $M'AM$ are of the form $X_1 \oplus X_2$. It follows that the eigenvectors of A are of the form

$$(2) \qquad M(X \oplus Y) = \frac{1}{\sqrt{2}} \begin{bmatrix} X_1 & X_2 \\ K_p X_1 & -K_p X_2 \end{bmatrix},$$

and thus the first $\frac{n}{2}$ (in this ordering) are symmetric and the next $\frac{n}{2}$ are skew-symmetric.

If n is odd we use $p = \frac{n-1}{2}$ and

$$(3) \qquad M_n = \frac{1}{\sqrt{2}} \begin{bmatrix} I_p & 0 & I_p \\ 0 & \sqrt{2} & 0 \\ K_p & 0 & -K_p \end{bmatrix},$$

and obtain $\lceil \frac{n}{2} \rceil = \frac{n+1}{2}$ symmetric and $\lfloor \frac{n}{2} \rfloor = \frac{n-1}{2}$ skew-symmetric eigenvectors $\qquad \square$

Result 9. The even and odd spectra of A are interlaced.

Proof. This actually follows from total postivity. But a proof in the Toeplitz context is in Delsarte and Genin [1983]. $\qquad \square$

Again, it is easy to see how the Toeplitz properties of A lead to horse-shoes. The eigenvector corresponding with the dominant eigenvalue is positive (and thus symmetric). All other eigenvectors will have both positive an negative elements. The next eigenvalue is odd and the third one is even, so plotting them in the plane will give a horseshoe. Throwing away the Perron-Frobenius solution and using the next two eigenvalues is very similar to double centering A and then computing the two dominant eigenvalues of $\tilde{A}$.

All the results in this subsection apply to Toeplitz matrices in general. This adds important information, because the classes of Toeplitz and TP matrices are quite different. Toeplitz matrices need not be non-negative and they need not even be positive semi-definite. There are many Toeplitz matrices that are not KMS. The covariance matrix of any weakly stationary sequence of random variables is Toeplitz, for example, so the same horseshoe result applies to covariance matrices of general ARMA models. Trench [1993] gives a sufficient condition for the interlacing of the even and odd spectra.

3.3. **A is a KMS Matrix.**

We get sign changes and interlacing eigenvector nodes from TP and we get interlacing symmetric and skew-symmetric eigenvectors from Toeplitz. If we use the precise form of the KMS matrix A we can get much more specific results.

3.3.1. *Inverse.*

The non-zero elements of $C = A^{-1}$ are

$$c_{11} = c_{nn} = \frac{1}{1 - \rho^2},$$

$$c_{i,i+1} = c_{i+1,i} = -\frac{\rho}{1 - \rho^2},$$

$$c_{22} = \cdots = c_{n-1,n-1} = \frac{1 + \rho^2}{1 - \rho^2}.$$

For this computation we could use Gantmacher and Krein [2002, p. 78, formula 29], but the result is classical and is easy to verify directly.

3.3.2. *Spectral.*

To solve the eigen-problem for A^{-1} we have to solve n equations. There are the $n - 2$ equations

(4a) $$-\rho x_k + (1 + \rho^2 - \mu)x_{k+1} - \rho x_{k+2} = 0,$$

for $k = 1, \cdots .n - 2$, which define the three-point recursion, and the two additional equations

(4b) $$(1 - \mu)x_1 - \rho x_2 = 0,$$

(4c) $$-\rho x_{n-1} + (1 - \mu)x_n = 0,$$

which define the boundary conditions.

Let's look first at the $n - 2$ equations (4a). We'll construct separate solutions corresponding to the even and odd spectra. If $\hat{x}_k = \cos(\alpha k + \beta)$ then

$$\rho(\hat{x}_k + \hat{x}_{k+2}) = \rho(\cos(\alpha k + \beta) + \cos(\alpha(k + 2) + \beta)) =$$
$$= 2\rho \cos(\alpha(k + 1) + \beta) \cos(\alpha) = 2\rho \cos(\alpha)\hat{x}_{k+1}.$$

Thus $\hat{x}$ is a solution to (4a) with $\mu = 1 + \rho^2 - 2\rho \cos(\alpha)$. Note that this implies $(1 - \rho)^2 \le \mu \le (1 + \rho)^2$.

We make $\hat{x}$ symmetric by choosing $\beta = -\frac{1}{2}\alpha(n + 1)$. This leaves the determination of α from (4b). Because of symmetry there is no need to consider (4c). We must have

$$(1 - \mu) \cos(\frac{1}{2}\alpha(n - 1)) = \rho \cos(\frac{1}{2}\alpha(n - 3)),$$

or

(5) $$\cos(\frac{1}{2}\alpha(n + 1)) - \rho \cos(\frac{1}{2}\alpha(n - 1)) = 0.$$

We have to find the $\lceil \frac{n}{2} \rceil$ solutions of this equation between zero and π. This must be done numerically.

For the odd spectrum we use $\hat{x}_k = \sin(\alpha(k - \frac{1}{2}(n + 1))$, which gives eigenvalues $\mu = 1 + \rho^2 - 2\rho \cos(\alpha)$. The boundary condition now is

$$(1 - \mu) \sin(\frac{1}{2}\alpha(n - 1)) = \rho \sin(\frac{1}{2}\alpha(n - 3)),$$

which can be written as

(6) $$\sin(\frac{1}{2}\alpha(n + 1)) - \rho \sin(\frac{1}{2}\alpha(n - 1)) = 0.$$

This equation has $\lfloor \frac{n}{2} \rfloor$ roots between zero and π, and these roots separate the roots of (5). We show an examples with $n = 10$ in Figure 1, for two different values of ρ.

Insert Figure 1 about here

It was shown by Grenander and Szegö [1958] that

(7) $$0 < \mu_1 < \frac{\pi}{n+1} < \mu_2 < \frac{2\pi}{n+1} < \cdots < \mu_n < \frac{n\pi}{n+1},$$

which is of course extremely helpful when solving numerically for the roots. In Figure 1 there is one red root between every two vertical red lines, and one green root between every two vertical green lines. The vertical red lines are at $2k\pi/(n+1)$ for $k = 1, \cdots, \lceil \frac{n}{2} \rceil$ and the vertical green lines are at $(2k+1)/(n+1)$ for $k = 1, \cdots, \lfloor \frac{n}{2} \rfloor$.

Appendix A has a program in R to rapidly compute the eigenvalues and eigenvectors. It uses the `uniroot()` function from the `stats` package, and is extremely fast, even for very large n. It is very similar, no doubt, to the BASIC program described by Trench [1988, p. 296].

Note that between zero and π the cosine decreases from $+1$ to -1. Thus the μ increase as a function of α, and are always between $(1 - \rho)^2$ and $(1 + \rho)^2$.

Of course the eigenvalues of A are of the form

$$\lambda_r(A) = \frac{1 - \rho^2}{1 + \rho^2 - 2\rho \cos(\alpha_r)}$$

where the α_r are the roots of (5) and (6). The eigenvectors are $\sin(\alpha_r(k - \frac{1}{2}(n+1)))$ for the odd spectrum and $\cos(\alpha_r(k - \frac{1}{2}(n+1)))$ for the even spectrum.

4. THE EFFECT OF CENTERING

Doubly centering the KMS matrix A to $\tilde{A} = J_n A J_n$ keeps the matrix positive semi-definite, but makes it singular. It destroys TP, and even TP(2). It also wreaks havoc on the Toeplitz property. Fortunately, a great deal can be salvaged. Remember that a square matrix C of order n is *centro-symmetric* if $c_{ij} = c_{n-i+1,n-j+1}$ for all i and j. Toeplitz matrices are special cases of centro-symmetric matrices. Equivalently, C is centro-symmetric if $C = K_n C K_n$ or, again equivalently, if $K_n C = C K_n$. We call a matrix C a *PCS matrix* if it has non-negative elements and is centro-symmetric.

Result 10. If C is centro-symmetric then $\tilde{C} = J_n C J_n$ is centro-symmetric.

Proof. It is easy to verify that $J_n K_n = K_n J_n = K_n - \frac{1}{n} e_n e_n'$. Thus $K_n \tilde{C} K_n = K_n J_n C J_n K_n = J_n K_n C K_n J_n = J_n C J_n = \tilde{C}$. □

Result 11. If C is centro-symmetric it has $\lceil \frac{n}{2} \rceil$ symmetric eigenvalues and $\lfloor \frac{n}{2} \rfloor$ skew-symmetric eigenvalues.

Proof. A very similar proof applies as for Toeplitz matrices [Cantoni and Butler, 1976]. A symmetric and centro-symmetric matrix C can be written, if n is even, as

$$C = \begin{bmatrix} C_1 & C_2 K_p \\ K_p C_2 & K_p C_1 K_p \end{bmatrix}$$

with both C_1 and C_2 symmetric of order p. For M defined by (1) we again have $M'CM = (C_1 + C_2) \oplus (C_1 - C_2)$, and thus the eigenvectors again have the form (2). For odd n we make the obvious adjustments. □

Result 12. If C is centro-symmetric the $\lfloor \frac{n}{2} \rfloor$ skew-symmetric eigenvectors of C are also eigenvectors of $\tilde{C} = JCJ$, with the same eigenvalues.

Proof. If $K_n x = -x$ then $e_n' K_n x = e_n' x = -e_n' x$. Thus $e_n' x = 0$ or $J_n x = x$. If $J_n x = x$ and $Cx = \lambda x$ then $\tilde{C} x = \lambda x$. □

What we have shown in this section is that the most important property of Toeplitz matrices from the perspective of horseshoes, which is that there are only symmetric and skew-symmetric eigenvectors, is preserved by centering. We now show that if even and odd eigenvalues are interlaced for a centr-symmetric matrix C, then they are interlaced for $J_n C J_n$.

Result 13. Suppose $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ are the eigenvalues of the positive semi-definite centro-symmetric matrix C and $\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \geq \cdots \geq \tilde{\lambda}_n = 0$ those of the double centered $\tilde{C} = J_n C J_n$. Suppose even and odd eigenvalues of C are interlaced. Then for n is even

even		*odd*		*even*		*odd*				*odd*		
λ_1	$\geq$	λ_2	$\geq$	λ_3	$\geq$	λ_4	$\geq$	$\cdots$	$>$	λ_n	$\geq$	0
		$\parallel$				$\parallel$				$\parallel$		
		$\tilde{\lambda}_1$	$\geq$	$\tilde{\lambda}_2$	$\geq$	$\tilde{\lambda}_3$	$\geq$	$\cdots$	$\geq$	$\tilde{\lambda}_{n-1}$	$\geq$	$\tilde{\lambda}_n = 0$

and for n is odd

even		*odd*		*even*		*odd*				*odd*		*even*		
λ_1	$\geq$	λ_2	$\geq$	λ_3	$\geq$	λ_4	$\geq$	$\cdots$	$\geq$	λ_{n-1}	$\geq$	λ_n	$\geq$	0
		$\parallel$				$\parallel$				$\parallel$				
$\tilde{\lambda}_1$	$\geq$	$\tilde{\lambda}_2$	$\geq$	$\tilde{\lambda}_3$	$\geq$	$\cdots$		$\geq$		λ_{n-2}	$\geq$	$\tilde{\lambda}_{n-1}$	$\geq$	$\tilde{\lambda}_n = 0$

Thus also for $\tilde{C}$ even and odd eigenvalues also interlace.

Proof. This combines the fact that the odd eigenvalues of C and $\tilde{C}$ are equal, with the interlacing result for eigenvalues given, for example, in Bellman [1960, Chapter 7, Theorem 5]. We know there is a $n \times (n-1)$ orthonormal matrix M such that $J_n = MM'$. Then the non-zero eigenvalues of J_nCJ_n are the eigenvalues of $M'CM$ and Bellman's result applies. Observe that we do not know the order of $\tilde{\lambda}_k$ and λ_{k+1} for k even. What we do know for even k is that $\lambda_k \geq \tilde{\lambda}_k \geq \lambda_{k+2}$. $\square$

Of course the elements of all eigenvectors of $\tilde{C}$, except for the last one, add up to zero. In particular the eigenvector corresponding with $\tilde{\lambda}_1$ is skew-symmetric, with only a single sign-change, and the eigenvector corresponding with $\tilde{\lambda}_2$ is symmetric. This is an essential component for what we need to have a horseshoe.

The lower bound λ_4 for $\tilde{\lambda}_2$ can be much improved for the non-negative centro-symmetric matrices C with interlaced even and odd eigenvalues, and a dominant even Perron-Frobenius eigenvalue.

Result 14. Suppose x is the symmetric eigenvalue of C corresponding with λ_3, and $\tilde{\lambda}_2$ is the dominant symmetric eigenvalue of $\tilde{C}$. Then $\tilde{\lambda}_2 \geq \lambda_3 - (\lambda_3 - \lambda_n)x'J_nx \geq \lambda_3(1 - x'J_nx)$.

Proof. Suppose $z = J_nx$, and $\epsilon^2 = (x - z)'(z - x) = 1 - x'J_nx$. Then z is symmetric and centered and thus

$$\tilde{\lambda}_2 \geq \frac{z'Az}{z'z} = \frac{(x + (z - x))'A(x + (z - x))'}{1 - \epsilon^2} \geq \frac{\lambda_3 - 2\lambda_3\epsilon^2 + \lambda_n\epsilon^2}{1 - \epsilon^2},$$

which is what we set out to prove. $\square$

Result 15. Suppose X are the $m = \lceil \frac{n}{2} \rceil$ symmetric eigenvectors of a centro-symmetric matrix C. Define $f = X'e_n$. Consider the "secular

equation"

$$F(\mu) = \sum_{i=1}^{m} \frac{f_i^2}{\lambda_i - \mu} = 0.$$

Then μ is a non-zero even eigenvalue of $\tilde{C} = J_n C J_n$ if and only if $F(\mu) = 0$. The corresponding eigenvector is $(C - \mu I)^{-1} e_n$.

Proof. Suppose $\tilde{C}\tilde{x} = \tilde{\lambda}\tilde{x}$. Then $J_n C \tilde{x} = \tilde{\lambda}\tilde{x}$ or $C\tilde{x} = \tilde{\lambda}\tilde{x} + \gamma e_n$ or $\tilde{x} = \gamma(C - \tilde{\lambda} I_n)^{-1} e_n$. This implies $e_n'(C - \tilde{\lambda} I_n)^{-1} e_n = 0$ or $F(\tilde{\lambda}) = 0$. Conversely if $F(\mu) = 0$ with $\mu \neq 0$ we define $\tilde{x} = (C - \mu I)^{-1} e_n$. Then $e_n'\tilde{x} = 0$ and $(C - \mu I_n)\tilde{x} = e_n$, and thus $\tilde{C}\tilde{x} = \mu\tilde{x}$. $\square$

The function $F(\mu)$ increases from $-\infty$ to $+\infty$ in every interval $\lambda_k < \mu < \lambda_{k+2}$, and thus it has a single root in each of these intervals. In Figure 2 we show $F(\mu)$ for the KMS matrix of order 0 with $\rho = \exp(-.1) = 0.9048$. Vertical red lines are the eigenvalues of A, vertical green lines those of $\tilde{A}$. At the green lines F is zero, at the red lines F has its vertical asymptotes

Insert Figure 2 about here

The secular equation $F(\mu) = 0$ can be used both for computational purposes and to derive bounds. For computations we refer, for example, to Melman [1995, 1997, 1998]. It is clear that with a efficient solver we can easily compute the roots of the double centered $\tilde{C}$ if we know those of the centro-symmetric C. We have already seen computing the roots of the KMS matrix A can be done efficiently, even for large n, and thus computing roots of $\tilde{A}$ can be done efficiently as well.

Appendix A. Code

```
 1  amat<-function(n,rho) {
 2  rho^outer(1:n,1:n,function(x,y) abs(x-y))
 3  }
 4
 5  imat<-function(n,rho) {
 6  x<-matrix(0,n,n)
 7  diag(x)<-1+rho^2
 8  x[1,1]<-1
 9  x[n,n]<-1
10  x<-x-rho*parDiag(10)
11  return(x/(1-rho^2))
12  }
13
14  doublyCenter<-function(x) {
15  n<-nrow(x)
16  s<-rowSums(x)/n
17  t<-sum(x)/(n^2)
18  return(x+t-outer(s,s,"+"))
19  }
20
21  secDiag<-function(n) {
22  outer(1:n,1:n,function(i,j) ifelse((i+j)==(n+1),1,0))
23  }
24
25  parDiag<-function(n) {
26  outer(1:n,1:n,function(i,j) ifelse(abs(i-j)==1,1,0))
27  }
28
29  bigMat<-function(n) {
30  mat<-matrix(0,n,n)
31  if ((n%%2)==0) {
32          p<-n/2
33          mat[1:p,1:p]<-diag(p)
34          mat[(p+1):n,(p+1):n]<--secDiag(p)
35          mat[1:p,(p+1):n]<-diag(p)
```

```r
36          mat[(p+1):n,1:p]<-secDiag(p)
37          mat<-mat/sqrt(2)
38          }
39 else {
40          p<-(n-1)/2
41          mat[1:p,1:p]<-diag(p)
42          mat[(p+2):n,(p+2):n]<--secDiag(p)
43          mat[1:p,(p+2):n]<-diag(p)
44          mat[(p+2):n,1:p]<-secDiag(p)
45          mat[p+1,p+1]<-sqrt(2)
46          mat<-mat/sqrt(2)
47          }
48 return(mat)
49 }
50
51 mkPlots<-function(n,rho) {
52          x<-seq(0,pi,length=100)
53          plot(x,cos(x*(n+1)/2)-rho*cos(x*(n-1)/2),type="l",
                 xlab="alpha",ylab="",lwd=3,col="RED")
54          lines(x,sin(x*(n+1)/2)-rho*sin(x*(n-1)/2),lwd=3,
                 col="GREEN")
55          abline(h=0)
56          for (i in 0:(n+1))
57           if (i%%2 == 0) abline(v=(i*pi)/(n+1),col="RED")
                   else abline(v=(i*pi)/(n+1),col="GREEN")
58 }
59
60 findRoots<-function(n,rho) {
61 feven<-function(x) cos(x*(n+1)/2)-rho*cos(x*(n-1)/2)
62 fodd<-function(x) sin(x*(n+1)/2)-rho*sin(x*(n-1)/2)
63 lbd<-rep(0,n); vec<-matrix(0,n,n); cv<-(1:n)-(n+1)/2
64 for (i in 1:ceiling(n/2)) {
65          int<-c(2*(i-1)*pi/(n+1),2*i*pi/(n+1))
66          rto<-uniroot(feven,int)$root
67          lbd[2*(i-1)+1]<-rto
68          vec[,2*(i-1)+1]<-cos(rto*cv)
```

```
69              }
70  for (i in 1:floor(n/2)) {
71              int<-c((2*i-1)*pi/(n+1),(2*i+1)*pi/(n+1))
72              rto<-uniroot(fodd,int)$root
73              lbd[2*i]<-rto
74              vec[,2*i]<-sin(rto*cv)
75              }
76  val<-(1-rho^2)/(1+rho^2-2*rho*cos(lbd))
77  vec<-vec/matrix(sqrt(colSums(vec^2)),10,10,byrow=TRUE)
78  return(list(values=val,vectors=vec))
79  }
```
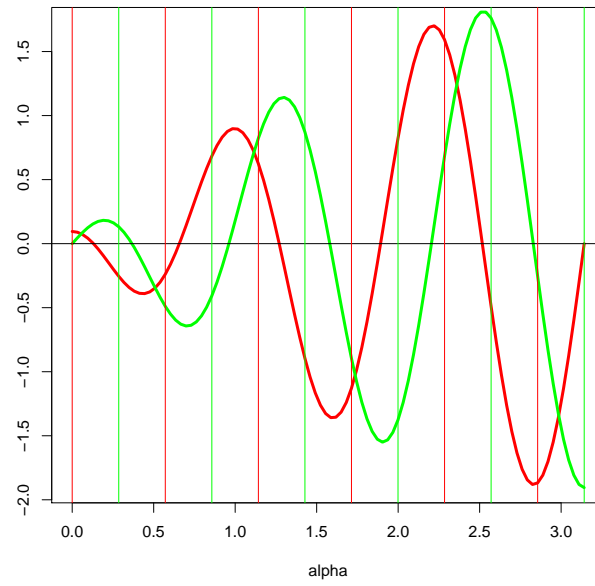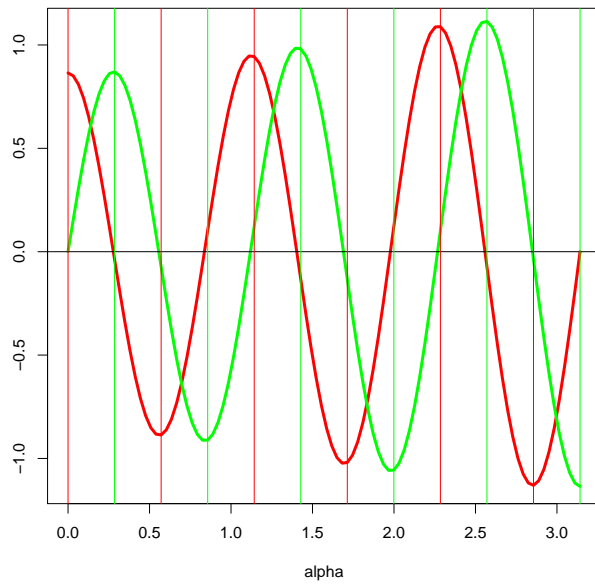
(a) $\sigma = 0.1, \rho = 0.9048$

(b) $\sigma = 2.0, \rho = 0.1353$

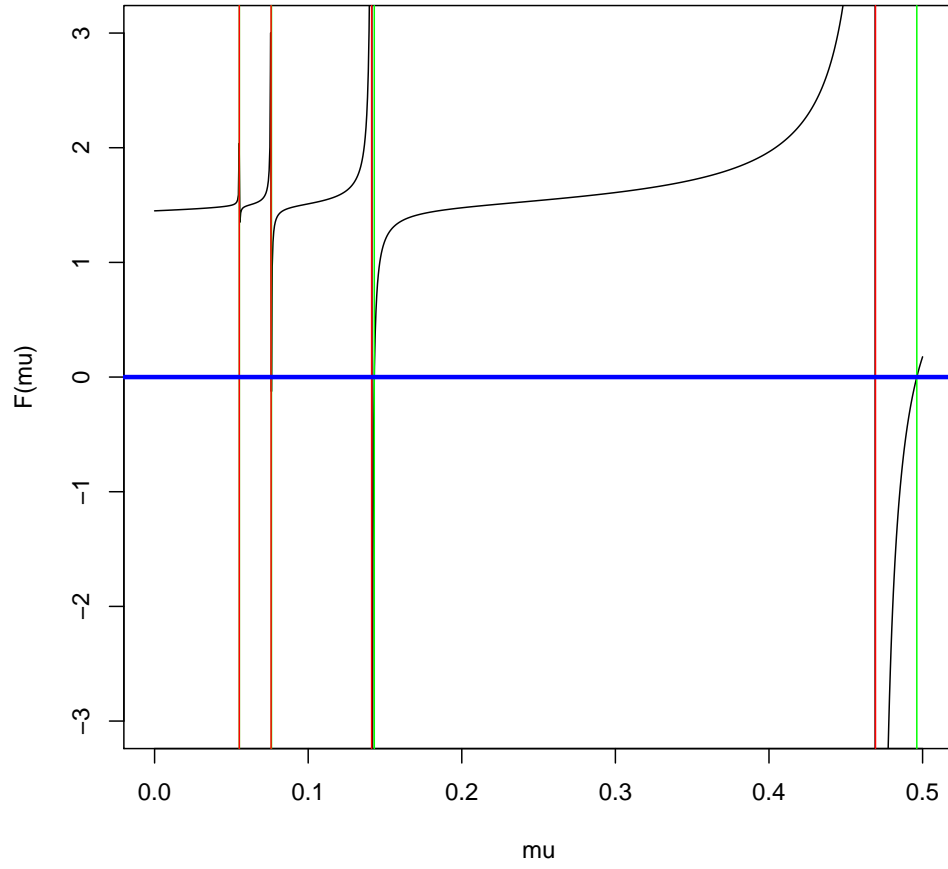FIGURE 1. Interlacing Roots for $n = 10$, red is even spectrum, green is odd spectrum

FIGURE 2. Roots of the Secular Equation

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