A NOTE ON THE GRCAR MATRIX

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1. Introduction. The Grcar type of matrix was devised in 1989 by Joseph F. Grcar to test some iterative methods [6]. For $n = 10$, the matrix is

$$G_{10} = \begin{pmatrix} 1 & 1 & 1 & 1 & & & & & & \\ -1 & 1 & 1 & 1 & 1 & & & & & \\ & -1 & 1 & 1 & 1 & 1 & & & & \\ & & -1 & 1 & 1 & 1 & 1 & & & \\ & & & -1 & 1 & 1 & 1 & 1 & & \\ & & & & -1 & 1 & 1 & 1 & 1 & \\ & & & & & -1 & 1 & 1 & 1 & 1 \\ & & & & & & -1 & 1 & 1 & 1 \\ & & & & & & & -1 & 1 & 1 \\ & & & & & & & & -1 & 1 \end{pmatrix}.$$

In fact, the matrix defined by Grcar was the transpose of that matrix, but this does not matter for our purposes. The matrix G_n of order n is Toeplitz upper Hessenberg and banded with -1 on the subdiagonal and 1 on the main diagonal and on three upper diagonals. It is often used for testing algorithms for computing eigenvalues since those of G_n are known to be sensitive to perturbations.

Being an unreduced upper Hessenberg matrix, G_n is nonderogatory, which means that its minimal polynomial is equal to its characteristic polynomial or equivalently all the eigenvalues are of geometric multiplicity one; see [5] for a proof. In this note we are interested in its determinant, its inverse, its LU factorization, and in a characterization of its asymptotic spectrum.

2. Determinant. We are interested in the determinants since they are involved in formulas for the inverses. There are recurrence formulas for the determinant of the successive Grcar matrices G_n. But, because of the banded structure of G_n, they are different for the first values of n.

PROPOSITION 2.1. *Let $d_n = \det(G_n)$. The determinants are*

$$\begin{aligned} d_1 &= 1, \\ d_2 &= d_1 + 1 = 2, \\ d_3 &= d_2 + d_1 + 1 = 4, \\ d_4 &= d_3 + d_2 + d_1 + 1 = 8, \\ d_n &= d_{n-1} + d_{n-2} + d_{n-3} + d_{n-4}, \ n \geq 5. \end{aligned}$$

Proof. This is obtained using the Laplace expansions from the first columns. ∎

The determinants are always positive, and increasing with n. Therefore, all the Grcar matrices are nonsingular. The first values are

$$1, \quad 2, \quad 4, \quad 8, \quad 15, \quad 29, \quad 56, \quad 108, \quad 208, \quad 401,$$

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for $n = 1, 2, \ldots, 10$. The value of the determinant is approximately multiplied by 2 when n is increased by 1. We have $\det(G_{100}) \approx 1.7944\ 10^{28}$ and $\det(G_{200}) \approx 5.6852\ 10^{56}$.

3. Inverse. Matrices G_n are persymmetric, that is, symmetric with respect to the principal anti-diagonal. The inverse of a persymmetric matrix is persymmetric. The inverse of G_n can be obtained as in [11] or [3]. However, we can compute it in a simpler way.

We first permute the rows of the matrix. Let P be the permutation matrix corresponding to moving the first row to the last position. We use the following result from [8].

PROPOSITION 3.1. *Let H be an unreduced upper Hessenberg matrix of order n such that*

$$PH = \begin{pmatrix} \widehat{H} & w \\ h^T & h_{1,n} \end{pmatrix},$$

where $\widehat{H}$ is square of order $n-1$. Let $\ell^T = h^T \widehat{H}^{-1}$ and $\alpha = h_{1,n} - \ell^T w \neq 0$. The inverse of PH is

$$(PH)^{-1} = \begin{pmatrix} \widehat{H}^{-1}(I + \frac{1}{\alpha} w \ell^T) & -\frac{1}{\alpha} \widehat{H}^{-1} w \\ -\frac{1}{\alpha} \ell^T & \frac{1}{\alpha} \end{pmatrix}$$

and

$$H^{-1} = \frac{1}{\alpha} \begin{pmatrix} -\widehat{H}^{-1} w & \widehat{H}^{-1}(\alpha I + w \ell^T) \\ 1 & -\ell^T \end{pmatrix}.$$

Proof. We use the LU factorization of PH, see [8]. We have

$$L = \begin{pmatrix} I & 0 \\ \ell^T & 1 \end{pmatrix} \Rightarrow L^{-1} = \begin{pmatrix} I & 0 \\ -\ell^T & 1 \end{pmatrix},$$

$$U = \begin{pmatrix} \widehat{H} & w \\ 0 & \alpha \end{pmatrix} \Rightarrow U^{-1} = \begin{pmatrix} \widehat{H}^{-1} & -\frac{1}{\alpha} \widehat{H}^{-1} w \\ 0 & \frac{1}{\alpha} \end{pmatrix}.$$

The result is obtained by $(PH)^{-1} = U^{-1} L^{-1}$. Note that the matrix $\hat{H}$ is upper triangular. □

We apply the previous result to the Grcar matrix. The diagonal entries of the matrix $\widehat{G}_n$ of order $n-1$ are equal to -1 and there are three upper diagonals with entries equal to 1. For instance, for $n = 10$,

$$\widehat{G}_{10} = \begin{pmatrix} -1 & 1 & 1 & 1 & 1 & & & & \\ & -1 & 1 & 1 & 1 & 1 & & & \\ & & -1 & 1 & 1 & 1 & 1 & & \\ & & & -1 & 1 & 1 & 1 & 1 & \\ & & & & -1 & 1 & 1 & 1 & 1 \\ & & & & & -1 & 1 & 1 & 1 \\ & & & & & & -1 & 1 & 1 \\ & & & & & & & -1 & 1 \\ & & & & & & & & -1 \end{pmatrix}.$$

First, we have to find what are the inverses of such Toeplitz upper triangular matrices.

Theorem 3.2. *The inverse of $\widehat{G}_n$ is a Toeplitz upper triangular matrix,*

$$(\widehat{G}_n)^{-1} = \begin{pmatrix} -1 & -d_1 & -d_2 & -d_3 & \cdots & -d_{n-3} & -d_{n-2} \\ & -1 & -d_1 & -d_2 & & -d_{n-4} & -d_{n-3} \\ & & -1 & \ddots & \ddots & \vdots & \vdots \\ & & & \ddots & \ddots & \vdots & \vdots \\ & & & & -1 & -d_1 & -d_2 \\ & & & & & -1 & -d_1 \\ & & & & & & -1 \end{pmatrix},$$

where the d_i's are the determinants of Proposition 2.1.

Proof. The proof is by induction. The result is clearly true for $\widehat{G}_1$, and also $\widehat{G}_2$. Let us assume that it holds for $\widehat{G}_{n-1}$. Since $\widehat{G}_n$ is an upper triangular matrix, the principal submatrix of order $n-1$ of $(\widehat{G}_n)^{-1}$ is $(\widehat{G}_{n-1})^{-1}$. So, we only have to consider the last column which is

$$(\widehat{G}_{n-1})^{-1} \begin{pmatrix} 0 & \cdots & 0 & 1 & 1 & 1 & 1 \end{pmatrix}^T, \tag{3.1}$$

and -1 as the last component. The components of the vector in (3.1) are the sums of the four last entries of each row of $(\widehat{G}_{n-1})^{-1}$. Using the definitions of the d_i's in Proposition 2.1 proves the claim. □

Let us compute the other quantities involved in Proposition 3.1. For the Grcar matrix,

$$h^T = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & \cdots & 0 \end{pmatrix},$$

and, for $n > 4$, w is a zero vector except for the last four components equal to 1. Therefore,

$$\begin{aligned} \ell^T &= h^T (\widehat{G}_n)^{-1}, \\ &= (-1, \quad -1-d_1, \quad -1-d_1-d_2, \quad -1-d_1-d_2-d_3, \quad d_1-d_2-d_3-d_4, \quad \cdots \\ &\quad - d_{n-5} - d_{n-4} - d_{n-3} - d_{n-2}), \\ &= (-d_1, \quad -d_2, \quad -d_3, \quad \cdots \quad -d_{n-1}). \end{aligned}$$

Since, for $n > 4$ $h_{1,n} = 0$, $\alpha = -\ell^T w$, that is, the sum of the last four components of $-\ell^T$, which yields $\alpha = d_n \neq 0$.

For $(\widehat{G}_n)^{-1} w$, we just have to compute the sum of the four last entries of each row of the matrix. It yields

$$(\widehat{G}_n)^{-1} w = \begin{pmatrix} -d_{n-1} & -d_{n-2} & \cdots & -d_2 & -d_1 \end{pmatrix}^T.$$

Theorem 3.3. *With the notation above and $n > 4$, the inverse of G_n is*

$$G_n^{-1} = \frac{1}{d_n} \begin{pmatrix} d_{n-1} & & & & & \\ d_{n-2} & & & & & \\ \vdots & & d_n (\widehat{G}_n)^{-1} + (\widehat{G}_n)^{-1} w \, \ell^T & & & \\ d_2 & & & & & \\ d_1 & & & & & \\ 1 & d_1 & d_2 & \cdots & \cdots & d_{n-2} & d_{n-1} \end{pmatrix}.$$

Proof. The proof is straightforward from Proposition 3.1 and the results above. Note that in the last row, we have the entries of the inverse, and not a product of determinants as it may look. ▯

Since $(\widehat{G}_n)^{-1}$ is upper triangular, we clearly see that the lower triangular part of G_n^{-1} is the lower triangular part of a rank-one matrix, as it is for all unreduced upper Hessenberg matrices. The first inverses are

$$G_2^{-1} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad G_3^{-1} = \frac{1}{4}\begin{pmatrix} 2 & -2 & 0 \\ 1 & 1 & -2 \\ 1 & 1 & 2 \end{pmatrix},$$

$$G_4^{-1} = \frac{1}{8}\begin{pmatrix} 4 & -4 & 0 & 0 \\ 2 & 2 & -4 & 0 \\ 1 & 1 & 2 & -4 \\ 1 & 1 & 2 & 4 \end{pmatrix}, \quad G_5^{-1} = \frac{1}{15}\begin{pmatrix} 8 & -7 & 1 & 2 & 4 \\ 4 & 4 & -7 & 1 & 2 \\ 2 & 2 & 4 & -7 & 1 \\ 1 & 1 & 2 & 4 & -7 \\ 1 & 1 & 2 & 4 & 8 \end{pmatrix}.$$

When the inverse of G_n is multiplied by its determinant, the entries are integers.

4. LU factorization. Linear systems with the matrix G_n can be solved using the factorization given in the proof of Proposition 3.1. However, it is also interesting to directly look for an LU factorization (without pivoting).

THEOREM 4.1. *The matrix G_n can be factorized as $G_n = L_n U_n$ with*

$$L_n = \begin{pmatrix} 1 & & & & & & & \\ -1 & 1 & & & & & & \\ & -\frac{d_1}{d_2} & 1 & & & & & \\ & & -\frac{d_2}{d_3} & 1 & & & & \\ & & & -\frac{d_3}{d_4} & 1 & & & \\ & & & & -\frac{d_4}{d_5} & 1 & & \\ & & & & & \ddots & \ddots & \\ & & & & & & -\frac{d_{n-2}}{d_{n-1}} & 1 \end{pmatrix},$$

where d_i is the determinant of the matrix G_i, and where the upper triangular matrix U_n has nonzero entries $u_{i,j}$ defined as

$$u_{1,1:4} = \begin{pmatrix} 1 & 1 & 1 & 1 \end{pmatrix},$$
$$u_{2,2:5} = \begin{pmatrix} \frac{d_2}{d_1} & \frac{d_3 - d_2}{d_1} & 1 + \frac{1}{d_1} & 1 \end{pmatrix}.$$

and, for $k \geq 3$,

$$u_{k,k} = \frac{d_k}{d_{k-1}},$$
$$u_{k,k+1} = \frac{d_{k+1} - d_k}{d_{k-1}}, \; k+1 \leq n,$$
$$u_{k,k+2} = 1 + \frac{d_{k-2}}{d_{k-1}}, \; k+2 \leq n,$$
$$u_{k,k+3} = 1, \; k+3 \leq n.$$

Proof. The proof is by induction. The result is clearly true for $n = 1, 2$. Let us assume that it holds for G_{n-1} and that

$$G_n = \begin{pmatrix} G_{n-1} & g_n \\ g_{n,n-1} e_{n-1}^T & 1 \end{pmatrix}.$$

L_n is a lower bidiagonal matrix and U_n is banded upper triangular. G_n can be factorized as

$$G_n = \begin{pmatrix} L_{n-1} & 0 \\ \ell_{n,n-1} e_{n-1}^T & 1 \end{pmatrix} \begin{pmatrix} U_{n-1} & u_n \\ 0 & u_{n,n} \end{pmatrix}.$$

By identification,

$$\begin{aligned} L_{n-1} U_{n-1} &= G_{n-1}, \\ L_{n-1} u_n &= g_n, \\ \ell_{n,n-1} &= \frac{g_{n,n-1}}{u_{n-1,n-1}}, \\ u_{n,n} &= g_{n,n} - \ell_{n,n-1} [u_n]_{n-1}. \end{aligned}$$

We have $g_{n,n-1} = -1$ and $g_{n,n} = 1$, and by the induction hypothesis, $u_{n-1,n-1} = d_{n-1}/d_{n-2}$. It yields $\ell_{n,n-1} = -d_{n-2}/d_{n-1}$. To obtain u_n we have to consider the inverse of L_{n-1} which is a lower bidiagonal matrix with a unit diagonal.

The inverse of a lower bidiagonal matrix B_n with a unit diagonal and values $\beta_1, \dots, \beta_{n-1}$ on the first subdiagonal is a lower triangular matrix,

$$B_n^{-1} = \begin{pmatrix} 1 & & & & \\ -\beta_1 & 1 & & & \\ \beta_1 \beta_2 & -\beta_2 & 1 & & \\ \vdots & \vdots & \vdots & \ddots & \\ (-1)^{n-1} \beta_1 \cdots \beta_{n-1} & (-1)^n \beta_2 \cdots \beta_{n-1} & \cdots & -\beta_{n-1} & 1 \end{pmatrix}.$$

Therefore,

$$L_{n-1}^{-1} = \begin{pmatrix} 1 & & & & & & & \\ 1 & 1 & & & & & & \\ \frac{1}{d_2} & \frac{d_1}{d_2} & 1 & & & & & \\ \frac{1}{d_3} & \frac{d_1}{d_3} & \frac{d_2}{d_3} & 1 & & & & \\ \frac{1}{d_4} & \frac{d_1}{d_4} & \frac{d_2}{d_4} & \frac{d_3}{d_4} & 1 & & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & & \\ \frac{1}{d_{n-2}} & \frac{d_1}{d_{n-2}} & \frac{d_2}{d_{n-2}} & \frac{d_3}{d_{n-2}} & \frac{d_4}{d_{n-2}} & \cdots & \frac{d_{n-3}}{d_{n-2}} & 1 \end{pmatrix}.$$

We have $g_n = \begin{pmatrix} 0 & \cdots & 0 & 1 & 1 & 1 \end{pmatrix}^T$. Since $u = u_n = L_{n-1}^{-1} g_n$, we have to sum the last three entries of the rows of L_{n-1}^{-1}. The first $n-4$ components are clearly 0. The last three ones are

$$\begin{aligned} u_{n-3} &= 1, \\ u_{n-2} &= 1 + \frac{d_{n-4}}{d_{n-3}} = \frac{d_n - d_{n-1} - d_{n-2}}{d_{n-3}}, \\ u_{n-1} &= 1 + \frac{d_{n-3} + d_{n-4}}{d_{n-2}} = \frac{d_n - d_{n-1}}{d_{n-2}}. \end{aligned}$$

We have

$$\ell_{n,n-1} = -\frac{1}{u_{n-1,n-1}} = -\frac{d_{n-2}}{d_{n-1}}.$$

Finally, since $g_{n,n} = 1$,

$$u_{n,n} = 1 + \frac{d_{n-2}}{d_{n-1}} \frac{d_n - d_{n-1}}{d_{n-2}} = \frac{d_n}{d_{n-1}},$$

which ends the proof. □

5. Eigenvalues. As far as we know, there is no explicit formula for the eigenvalues of Grcar matrices. In 1985, W.F. Trench published a characterization of the eigenvalues of banded Toeplitz matrices [12]. Let us specialize his results to our matrices G_n. Let

$$q(z, \lambda) = z^4 + z^3 + z^2 + (1 - \lambda)z - 1, \tag{5.1}$$

be the polynomial defined by the symbol of $G_n - \lambda I$ after multiplication by z. For a given λ, the polynomial $q(z, \lambda)$ has distinct roots except for at most four values of λ. This is obtained by considering the resultant of $q(z, \lambda)$ and its derivative with respect to z. It is a 7×7 determinant that must be zero if there is a multiple root. Let $\gamma = 1 - \lambda$. The resultant is the polynomial

$$r(\gamma) = -27\gamma^4 + 14\gamma^3 - 141\gamma^2 - 130\gamma - 279.$$

It has four distinct roots (2 complex pairs) which gives four distinct values of λ,

$$7.0708\ 10^{-2} \pm 2.2635\, i, \quad 1.6700 \pm 1.1301\, i.$$

Hence, the generic case is that $q(z, \lambda) = 0$ has four distinct solutions z_i, $i = 1, \dots, 4$. Let

$$Z_n = \begin{pmatrix} 1 & 1 & 1 & 1 \\ z_1^{n+1} & z_2^{n+1} & z_3^{n+1} & z_4^{n+1} \\ z_1^{n+2} & z_2^{n+2} & z_3^{n+2} & z_4^{n+2} \\ z_1^{n+3} & z_2^{n+3} & z_3^{n+3} & z_4^{n+3} \end{pmatrix},$$

whose entries are functions of λ. Trench proved that λ is in the spectrum of G_n if and only if $\det(Z_n) = 0$. Moreover, if y is in the null space of Z_n, that is, with $Z_n y = 0$, an eigenvector x related to λ can be written as

$$x_i = \sum_{j=1}^{4} y_j z_j^i, \quad i = 1, \dots, n.$$

Even though the solutions z_i of the quartic equation $q(z, \lambda) = 0$ can be written with radicals, their expressions as functions of λ or $\gamma = 1 - \lambda$ are too much intricate to be useful for obtaining an analytic formula for the eigenvalues. Hence, the previous result has only a theoretical interest.

Figure 5.1 displays the eigenvalues of G_n for $n = 5, 10, 20, 100$. We see that, at least when n is large, the eigenvalues of G_n are located on well-defined curves and there is some kind of convergence. This motivates the study of the asymptotic spectrum. Asymptotically, the spectrum is composed of three curves. The lower left curve is the symmetric with respect to the x-axis of the upper left curve.

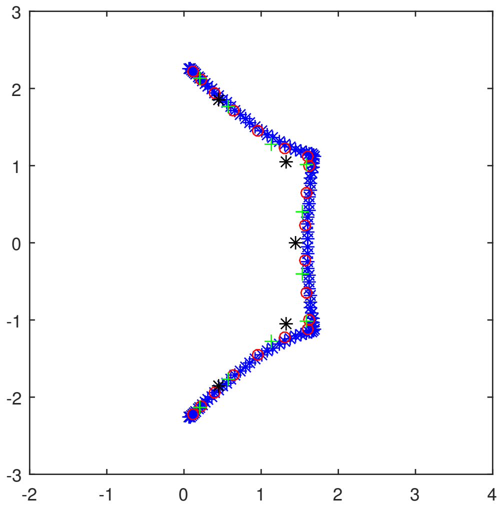

FIG. 5.1. *Eigenvalues of Grcar matrices G_n, $n = 5$ (black *), $n = 10$ (green +), $n = 20$, (red o), $n = 100$, (blue *)*

6. The asymptotic spectrum. The limit of spectra of Toeplitz matrices was investigated by P. Schmidt and F. Spitzer [10] in 1960. They introduced the concept of asymptotic spectrum. Let T_n be a Toeplitz matrix of order n with a spectrum

$$\Sigma_n = \{\lambda \,|\, \det(T_n - \lambda I) = 0\}.$$

The asymptotic spectrum is defined as

$$\Sigma_a = \{\lambda \,|\, \lambda = \lim_{m\to\infty} \lambda_m,\ \lambda_m \in \Sigma_{\ell_m}, \lim_{m\to\infty} \ell_m = \infty\}.$$

Hence, there is, at least, a subsequence of spectra converging in some sense to the asymptotic spectra. In general, Σ_n is not contained in Σ_a for all values of n.

Let p and q two integers defining the bandwidth of T_n. For G_n, $p = 1$ and $q = 3$. If the entries of a generic row of T_n are

$$t_p, \ldots, t_0, t_1, \ldots, t_q,$$

t_0 being the diagonal entry, an eigenvalue λ and the corresponding eigenvector x must satisfy

$$\sum_{\ell=-p}^{q} t_\ell x_{j+\ell} = \lambda x_j, \quad j = 1, 2, \ldots, n, \tag{6.1}$$

with boundary conditions

$$x_{-\ell} = 0,\ \ell = 0, 1, \ldots, p-1, \quad x_{n+\ell} = 0,\ \ell = 1, 2, \ldots, q.$$

Relation (6.1) is a difference equation for x. We can look for a solution with $x_j = z^j$ where z is a complex number. Then, from (6.1), we have

$$\lambda = \sum_{\ell=-p}^{q} t_\ell z^\ell. \tag{6.2}$$

For a given λ, equation (6.2) has $p+q$ roots $z_i(\lambda)$ ordered such that

$$|z_1(\lambda)| \le |z_2(\lambda)| \le \cdots \le |z_{p+q}(\lambda)|.$$

In [10] it is proved that the asymptotic spectrum is characterized as

$$\Sigma_a = \{\lambda \mid |z_p(\lambda)| = |z_{p+1}(\lambda)|\}. \tag{6.3}$$

Schmidt and Spitzer proved that Σ_a is not empty, has no isolated point, and consists of a finite number of analytic arcs. However, they did not prove that it is connected. This was proved by J.L. Ullman [13]. I.I. Hirschman Jr. [7] proved that Σ_a can be represented as a finite union of closed analytic arcs, where either distinct arcs are disjoint, or, if not, their intersection consists of one or both common end points. He studied the limiting eigenvalue distribution. He showed that there exists a probability measure μ on Σ_a such that

$$\frac{1}{n} \sum_{\lambda \in \Sigma_n} \delta_\lambda \to \mu,$$

where each eigenvalue in the sum is counted according to its multiplicity. Details on spectral properties of banded Toeplitz matrices can be found in the book [2]; for a generalization, see also [4].

For G_n, (6.3) means that Σ_a is the set of λ's in the complex plane such that the two roots of

$$\lambda = -\frac{1}{z} + 1 + z + z^2 + z^3. \tag{6.4}$$

with the two smallest moduli have the same modulus. Since the entries of G_n are real, Σ_a is symmetric with respect to the x-axis. Equation (6.4) can be converted into a polynomial equation of degree 4 in z or $1/z$. Note that this polynomial is the same as $q(z,\lambda)$ defined in (5.1).

In [1], R.M. Beam and R.F. Warming proposed an algorithm for computing points on the asymptotic spectrum of a banded Toeplitz matrix.

Let us briefly explain their algorithm on our example. We write $z = \widehat{z}\, e^{-i\phi}$ with $0 < \phi < \pi$. Since $\widehat{z}\, e^{i\phi}$ must give the same value of λ, by subtracting, we obtain

$$\sin(\phi)\frac{1}{\widehat{z}} + \sin(\phi)\widehat{z} + \sin(2\,\phi)\widehat{z}^2 + \sin(3\,\phi)\widehat{z}^3 = 0.$$

It is somehow easier to work with $y = 1/\widehat{z}$ for which we obtain

$$y^4 + y^2 + \frac{\sin(2\,\phi)}{\sin(\phi)} y + \frac{\sin(3\,\phi)}{\sin(\phi)} = 0.$$

But, $\sin(2\,\phi) = 2\,\sin(\phi)\,\cos(\phi)$ and $\sin(3\,\phi) = 3\,\sin(\phi) - 4\,\sin^3(\phi)$. Therefore, defining $\zeta = \cos(\phi)$, the equation becomes

$$y^4 + y^2 + 2\,\zeta\, y - 1 + 4\,\zeta^2 = 0. \tag{6.5}$$

This is a depressed quartic equation (which means that the coefficient of y^3 is zero). The nature of the roots (real or complex) depends on the sign of the discriminant Δ which is

$$\Delta(\zeta) = 16384\zeta^6 - 12464\zeta^4 + 3568\zeta^2 - 400.$$

This is a function of ζ which is symmetric with respect to the vertical axis. The limit when ζ goes to $-\infty$ or $+\infty$ is $+\infty$. It has only two real zeros, symmetric with respect to 0, one negative ζ_- and one positive ζ_+ which is approximately 0.5623291174585. It corresponds to an angle which is a little less than 56 degrees. The function is decreasing for $\zeta < 0$ and increasing when $\zeta > 0$. The discriminant $\Delta(\zeta)$ is negative when $\zeta \in (\zeta_-, \zeta_+)$, and positive outside. It implies that the equation (6.5) has two complex conjugate pairs of roots when $\Delta(\zeta) > 0$ (that is, for angles between 0 and 56 degrees) and two distinct real roots and a complex pair when $\Delta(\zeta) < 0$.

For each root of equation (6.5), and using (6.4), we compute λ (which is a function of ζ) and the solutions of

$$y^4 + (\lambda - 1)y^3 - y^2 - y - 1 = 0.$$

By definition, this equation has at least two roots of equal modulus. If the roots with the two largest moduli have the same modulus, λ is a point of the asymptotic spectrum. This is done with as many values of $\zeta \in (-1, 1)$ as we wish. In fact, it is clear that it is enough to consider the interval $(0, 1)$.

Now, we will show that we can obtain an analytic description of the asymptotic spectrum of the Grcar matrices. Let us look for the solution of equation (6.5). We first consider the case $\Delta(\zeta) > 0$, that is, $\zeta > \zeta_+$. We have two pairs of complex conjugate roots.

LEMMA 6.1. *Let ζ be such that $\Delta(\zeta) > 0$. The four solutions of equation (6.5) can be written as*

$$r + \imath s_1, \quad r - \imath s_1, \quad -r + \imath s_2, \quad -r - \imath s_2,$$

with $r = \sqrt{\widehat{r}}$. Let α, β, and γ defined as

$$\alpha = \frac{11}{144} - \frac{\zeta^2}{3}, \quad \beta = \frac{111}{5184} - \frac{5\,\zeta^2}{96}, \quad \gamma = \alpha^3 + \beta^2. \tag{6.6}$$

Then,

$$\widehat{r} = 2\sqrt{-\alpha}\,\cos\left(\frac{1}{3}\arccos\left(\frac{\beta}{(-\alpha)^{\frac{3}{2}}}\right)\right) - \frac{1}{6},$$

and

$$s_1 = \sqrt{\frac{1}{2}\left(1 + 2\widehat{r} + \frac{\zeta}{r}\right)}.$$

Proof. We can assume that the solutions have this form because the coefficient of y^3 in (6.5) is zero. Taking the product of the four roots and by identification with the coefficients of the polynomial of equation (6.5), we have the three following equations,

$$\begin{aligned}
(A) \quad & (r^2 + s_1^2) + (r^2 + s_2^2) = 1 + 4r^2, \\
(B) \quad & (r^2 + s_1^2) - (r^2 + s_2^2) = \frac{\zeta}{r}, \\
(C) \quad & (r^2 + s_1^2)\,(r^2 + s_2^2) = 4\zeta^2 - 1.
\end{aligned}$$

Clearly, we need to have $1 \geq \zeta \geq 1/2$ which is satisfied with our hypothesis on ζ. Using (A)+(B), (A)-(B), and (C), we obtain an equation for r,

$$16r^6 + 8r^4 + (5 - 16\zeta^2)r^2 - \zeta^2 = 0. \tag{6.7}$$

Defining $\widehat{r} = r^2$, we obtain a cubic polynomial equation that we can solve for $\widehat{r}$ as a function of ζ. If there is a positive real root, since we are looking for $r \geq 0$, we take $r = \sqrt{\widehat{r}}$, and

$$2s_1^2 = 1 + 2r^2 + \frac{\zeta}{r}, \quad 2s_2^2 = 1 + 2r^2 - \frac{\zeta}{r}.$$

Note that if r is changed to $-r$, s_1 becomes s_2 and vice-versa. Clearly, $s_1^2 > s_2^2$ and the largest modulus of the roots is given by $r \pm i\, s_1$. Let us now solve the cubic equation for $\widehat{r}$ divided by the leading coefficient 16. We have a polynomial of degree 3 with coefficients

$$a_3 = 1, \quad a_2 = \frac{1}{2}, \quad a_1 = \frac{5}{16} - \zeta^2, \quad a_0 = -\frac{\zeta^2}{16}.$$

The number of real solutions depends on the sign of γ defined in (6.6). As a function of ζ, γ is monotonely decreasing on $[1/2, 1]$ and has a unique zero for ζ_+.

Since, with our hypothesis on ζ, $\gamma \leq 0$, there are three real solutions of the equation for $\widehat{r}$. Note that it implies that $\alpha \leq 0$. Let $\eta = 2\sqrt{-\alpha}$, and

$$\theta = \arccos\left(\frac{\beta}{(-\alpha)^{\frac{3}{2}}}\right), \quad \varphi_1 = \frac{\theta}{3}, \quad \varphi_2 = \varphi_1 - \frac{2\pi}{3}, \quad \varphi_3 = \varphi_1 + \frac{2\pi}{3}.$$

Then, the three solutions are

$$\widehat{r}_i = \eta \cos(\varphi_i) - \frac{1}{6}.$$

We must pick a positive root to compute r and, then, s_1 and s_2 as above. It is given by $\widehat{r}_1$. The solution we will be interested in later on is $r - is_1$, where

$$\widehat{r} = 2\sqrt{\frac{\zeta^2}{3} - \frac{11}{144}} \cos\left(\frac{1}{3} \arccos\left(\frac{\frac{111}{5184} - \frac{5\,\zeta^2}{96}}{\left(\frac{\zeta^2}{3} - \frac{11}{144}\right)^{\frac{3}{2}}}\right)\right) - \frac{1}{6}.$$

The cosine is positive as well as $\widehat{r}$, and

$$r = \sqrt{\widehat{r}}, \quad s_1 = \sqrt{\frac{1}{2}\left(1 + 2\widehat{r} + \frac{\zeta}{r}\right)}.$$

□

Now, we consider the case $\Delta(\gamma) \leq 0$, that is $\zeta \in (0, \zeta_+]$ and show that we obtain the same equation (6.7) for r. We already know that we have two distinct real roots and a pair of complex conjugate roots if $\zeta < \zeta_+$. Therefore, the two solutions with the same modulus are those of the complex pair. If $\zeta = \zeta_+$, the two real solutions are equal. We will see that their modulus is smaller than the moduli of the roots in the complex pair.

LEMMA 6.2. *Let ζ be such that $\Delta(\zeta) \leq 0$. The four solutions of equation (6.5) can be written as*

$$r + \imath s, \quad r - \imath s, \quad r_1, \quad r_2,$$

with r, s, r_1, and r_2 real. Then, the real part r is a solution of equation (6.7).

Let α, β, γ defined by (6.6), and $\delta = (|\beta| + \sqrt{\gamma})^{1/3}$. Then, $r = \sqrt{\widehat{r}}$ with

$$\widehat{r} = \begin{cases} \delta - \frac{\alpha}{\delta} - \frac{1}{6} & \text{if } \beta \geq 0\,, \\ \frac{\alpha}{\delta} - \delta - \frac{1}{6} & \text{if } \beta < 0 \end{cases}$$

and $s = \sqrt{\frac{1}{2}\left(1 + 2\widehat{r} + \frac{\zeta}{r}\right)}$

Proof. We write the equation (6.5) as

$$[y^2 - 2ry + r^2 + s^2]\,[y^2 - (r_1 + r_2)y + r_1 r_2] = 0.$$

By identification of the coefficients of y^3 and y^2, we obtain

$$r_1 + r_2 = -2r,$$
$$r_1\, r_2 = 1 + 3r^2 - s^2.$$

It yields

$$[y^2 - 2ry + r^2 + s^2]\,[y^2 + 2ry + 1 + 3r^2 - s^2] = 0.$$

With the coefficient of y and the constant term, we get

$$-r\,(1 + 3r^2 - s^2) + r\,(r^2 + s^2) = \zeta,$$
$$(r^2 + s^2)\,(1 + 3r^2 - s^2) = 4\zeta^2 - 1.$$

Multiplying the second equation with r^2, we have the difference and the product of two quantities $\tilde{\alpha} = r(1 + 3r^2 - s^2)$ and $\tilde{\beta} = r(r^2 + s^2)$. We also have $\tilde{\alpha} + \tilde{\beta} = r + 4r^3$. Eliminating $\tilde{\beta}$, we obtain a quadratic equation for $\tilde{\alpha}$,

$$\tilde{\alpha}^2 + \zeta\,\tilde{\alpha} + r^2(1 - 4\zeta^2) = 0.$$

It yields $\tilde{\alpha} + \tilde{\beta} = r + 4r^3 = \pm\sqrt{(1 + 16r^2)\zeta^2 - 4r^2}$. Squaring this relation, we obtain

$$(r + 4r^3)^2 = (1 + 16r^2)\zeta^2 - 4r^2.$$

Simplifying, we have a polynomial equation for r,

$$16r^6 + 8r^4 + (5 - 16\zeta^2)r^2 - \zeta^2 = 0,$$

which is the same as (6.7). Moreover, we obtain

$$s^2 = r^2 + \frac{\zeta}{r} + \frac{1}{2},$$

which is the same as s_1^2 in Lemma 6.1. Here, the cubic equation for $\widehat{r}$ has only one real solution which is given in the statement of the lemma. □

If $\zeta = \zeta_+$, we have $r_1 = r_2 = -r$. It yields $r^2 + s^2 = 1 + 3r^2$, and the complex conjugate solution gives the largest modulus.

To obtain the upper part (above the x-axis) of the asymptotic spectrum, we use the solution $r - i\,s$ described in lemmas 6.1 and 6.2, with $s = s_1$ when $\Delta(\gamma) > 0$. We have to multiply with $e^{i\phi} = \zeta + i\sqrt{1-\zeta^2}$ to get

$$\frac{1}{z} = \tilde{y} = (r\,\zeta + s\,\sqrt{1-\zeta^2}) + i\,(-s\,\zeta + r\,\sqrt{1-\zeta^2}). \tag{6.8}$$

Note that we have $|\tilde{y}|^2 = r^2 + s^2$. Lemmas 6.1 and 6.2 lead to the following result.

THEOREM 6.3.
Let $\zeta \in (0,1)$. With the notation above and (6.8), let

$$\sin(\varphi) = \frac{-s\,\zeta + r\,\sqrt{1-\zeta^2}}{\sqrt{r^2+s^2}} < 0, \quad \cos(\varphi) = \frac{r\,\zeta + s\,\sqrt{1-\zeta^2}}{\sqrt{r^2+s^2}} > 0.$$

The points λ on the upper part of the asymptotic spectrum of G_n are given by

$$\begin{aligned} Re(\lambda) &= 1 - \frac{1}{|\tilde{y}|^2} + \frac{\cos(\varphi)}{|\tilde{y}|}\left[1 - |\tilde{y}|^2 + \frac{2\cos(\varphi)}{|\tilde{y}|} + \frac{4\cos^2(\varphi) - 3}{|\tilde{y}|^2}\right], \\ Im(\lambda) &= -\frac{\sin(\varphi)}{|\tilde{y}|}\left[1 + |\tilde{y}|^2 + \frac{2\cos(\varphi)}{|\tilde{y}|} + \frac{3 - 4\sin^2(\varphi)}{|\tilde{y}|^2}\right], \end{aligned}$$

with $\tilde{y}$ defined by (6.8).

Proof. The point λ on the upper part of the asymptotic spectrum is

$$\lambda = -\tilde{y} + 1 + \frac{1}{\tilde{y}} + \frac{1}{\tilde{y}^2} + \frac{1}{\tilde{y}^3}.$$

To compute λ, we use the polar form of $\tilde{y} = |\tilde{y}|\,e^{i\varphi}$, with

$$|\tilde{y}|^2 = r^2 + s^2, \quad \varphi = \mathrm{atan2}(-s\,\zeta + r\,\sqrt{1-\zeta^2}, r\,\zeta + s_1\,\sqrt{1-\zeta^2}).$$

Then, $\tilde{y}^j = |\tilde{y}|^j\,e^{ij\varphi} = |\tilde{y}|^j\,(\cos(j\varphi) + i\,\sin(j\varphi))$. For our case the values $-s\,\zeta + r\,\sqrt{1-\zeta^2}$ are negative, and thus

$$\sin(\varphi) = \frac{-s\,\zeta + r\,\sqrt{1-\zeta^2}}{\sqrt{r^2+s^2}} < 0, \quad \cos(\varphi) = \frac{r\,\zeta + s\,\sqrt{1-\zeta^2}}{\sqrt{r^2+s^2}} > 0.$$

Moreover,

$$\sin(2\varphi) = 2\sin(\varphi)\,\cos(\varphi), \quad \cos(2\varphi) = 2\cos^2(\varphi) - 1,$$

$$\sin(3\varphi) = 3\sin(\varphi) - 4\sin^3(\varphi), \quad \cos(3\varphi) = 4\cos^3(\varphi) - 3\cos(\varphi).$$

It yields, as functions of ζ,

$$\begin{aligned} \mathrm{Re}(\lambda) &= -|\tilde{y}|\,\cos(\varphi) + 1 + \frac{\cos(\varphi)}{|\tilde{y}|} + \frac{\cos(2\varphi)}{|\tilde{y}|^2} + \frac{\cos(3\varphi)}{|\tilde{y}|^3}, \\ \mathrm{Im}(\lambda) &= -|\tilde{y}|\,\sin(\varphi) - \frac{\sin(\varphi)}{|\tilde{y}|} - \frac{\sin(2\varphi)}{|\tilde{y}|^2} - \frac{\sin(3\varphi)}{|\tilde{y}|^2}. \end{aligned}$$

Rearranging the terms, we obtain

$$\begin{aligned}\mathrm{Re}(\lambda) &= 1 - \frac{1}{|\tilde y|^2} + \frac{\cos(\varphi)}{|\tilde y|}\left[1 - |\tilde y|^2 + \frac{2\cos(\varphi)}{|\tilde y|} + \frac{4\cos^2(\varphi) - 3}{|\tilde y|^2}\right],\\ \mathrm{Im}(\lambda) &= -\frac{\sin(\varphi)}{|\tilde y|}\left[1 + |\tilde y|^2 + \frac{2\cos(\varphi)}{|\tilde y|} + \frac{3 - 4\sin^2(\varphi)}{|\tilde y|^3}\right].\end{aligned}$$

This is a parametric description of the upper part of the asymptotic spectra of G_n for $\zeta \in (0, 1]$. The lower part is obtained by changing the sign of the imaginary part. ☐

Theorem 6.3 shows that the expression of the asymptotic spectrum of G_n is a complicated function of ζ. However, the real and imaginary parts are very smooth functions of ζ and they can be fitted with least squares polynomials or a rational approximation.

An good approximation can be obtained using rational functions. We use the AAA algorithm of Nakatsukasa, Sète, and Trefethen [9]. Sets of 100 function values on $[10^{-2}, 1]$ are approximated by a rational function

$$r(\zeta) = \frac{\sum_{j=1}^{m} \frac{w_j f_j}{\zeta - z_j}}{\sum_{j=1}^{m} \frac{w_j}{\zeta - z_j}}.$$

We asked for an accuracy of 10^{-10}. It yields $m = 14$ for the real part and $m = 15$ for the imaginary part. For the real part, the weights w_j are

$$\begin{aligned}&-4.6364\ 10^{-1},\ 5.4008\ 10^{-2},\ 3.4071\ 10^{-2},\ -1.2689\ 10^{-1},\ -4.6563\ 10^{-2},\\ &3.6930\ 10^{-1},\ 3.3729\ 10^{-2},\ 2.5439\ 10^{-1},\ -2.7119\ 10^{-2},\ -4.6470\ 10^{-1},\\ &5.8926\ 10^{-2},\ -8.7516\ 10^{-2},\ 5.5798\ 10^{-1},\ -1.4597\ 10^{-1}.\end{aligned}$$

The values f_j of the data are

$$\begin{aligned}&7.0708\ 10^{-2},\ 1.6955,\ 1.6181,\ 3.9119\ 10^{-1},\ 1.2370,\ 1.6575,\ 1.4835\\ &1.6316,\ 1.6468,\ 1.6438,\ 8.8905\ 10^{-1},\ 1.6196,\ 1.0637\ 10^{-1},\ 1.6802.\end{aligned}$$

The support points z_j in $[10^{-2}, 1]$ are

$$\begin{aligned}&1.0000,\ 4.2000\ 10^{-1},\ 1.0000\ 10^{-2},\ 9.1000\ 10^{-1},\ 6.7000\ 10^{-1},\ 2.8000\ 10^{-1},\\ &5.9000\ 10^{-1},\ 1.7000\ 10^{-1},\ 5.1000\ 10^{-1},\ 2.3000\ 10^{-1},\ 7.7000\ 10^{-1},\\ &6.0000\ 10^{-2},\ 9.9000\ 10^{-1},\ 3.5000\ 10^{-1}.\end{aligned}$$

For the imaginary part, the weights w_j are

$$\begin{aligned}&8.1519\ 10^{-4},\ 2.3012\ 10^{-2},\ 9.6495\ 10^{-2},\ 1.0884\ 10^{-2},\ -6.3678\ 10^{-2},\\ &-1.0310\ 10^{-1},\ -1.2201\ 10^{-2},\ 2.4750\ 10^{-2},\ 6.4215\ 10^{-1},\ -4.9020\ 10^{-3},\\ &-4.9754\ 10^{-1},\ 2.6857\ 10^{-1},\ -2.2893\ 10^{-1},\ 2.2010\ 10^{-1},\ -3.7642\ 10^{-1}.\end{aligned}$$

The values f_j of the data are

$$\begin{aligned}&2.2635,\ 3.0810\ 10^{-2},\ 9.3667\ 10^{-1},\ 1.5961,\ 1.2240,\ 1.8451\ 10^{-1},\ 1.1438,\ 1.1808,\\ &7.3986\ 10^{-1},\ 1.8618,\ 8.1797\ 10^{-1},\ 1.2878,\ 1.3039,\ 3.6679\ 10^{-1},\ 5.7302\ 10^{-1}.\end{aligned}$$

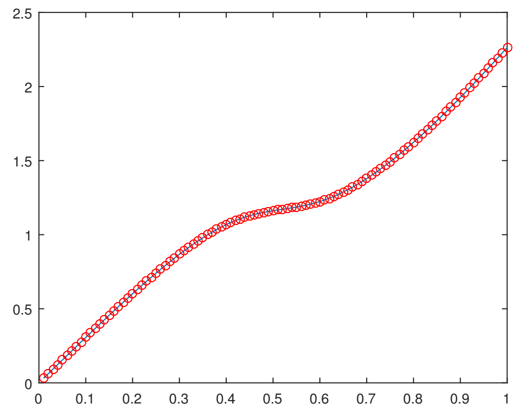

FIG. 6.1. *Imaginary part of the asymptotic spectrum (blue) and rational fit (red o)*

The support points z_j in $[10^{-2}, 1]$ are

$$1.0000,\ 1.0000\ 10^{-2},\ 3.3000\ 10^{-1},\ 7.9000\ 10^{-1},\ 6.0000\ 10^{-1},\ 6.0000\ 10^{-2},$$
$$4.7000\ 10^{-1},\ 5.4000\ 10^{-1},\ 2.5000\ 10^{-1},\ 8.8000\ 10^{-1},\ 2.8000\ 10^{-1},\ 6.5000\ 10^{-1},$$
$$6.6000\ 10^{-1},\ 1.2000\ 10^{-1},\ 1.9000\ 10^{-1}.$$

The relative errors are of the order of 10^{-11} or smaller; see Figure 6.1.

Figure 6.2 shows the asymptotic spectrum, computed with the formulas of Theorem 6.3, and the eigenvalues of G_{500} computed with the `eig` Matlab function. The eigenvalues must be close to the asymptotic spectrum, but we see that this is not always true for all the eigenvalues. It means that the QR algorithm has difficulties computing accurate eigenvalues for this matrix when n is large. In [1], Beam and Warming proposed a scaling of the matrix to improve the computation of the spectra of banded Toeplitz matrices, but it requires the computation of the asymptotic spectrum.

7. Conclusion. We have studied the Grcar matrices giving formulas for computing the determinants, the inverses, and the LU factorizations. We also showed how to obtain a parametric description of the asymptotic spectrum. This could be useful when testing eigenvalue solvers with Grcar matrices of large dimension.

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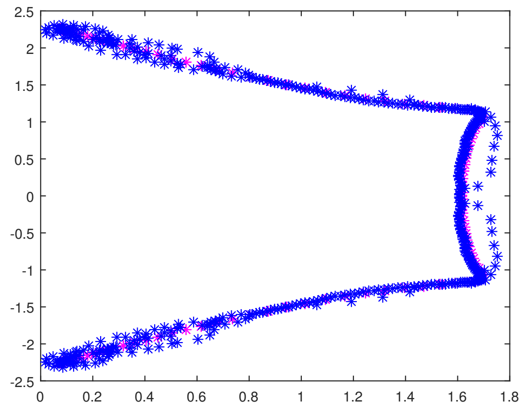

FIG. 6.2. *Eigenvalues of the Grcar matrix G_{500} (blue *) and asymptotic spectrum (magenta *)*

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