NULLITIES FOR A CLASS OF 0-1 SYMMETRIC TOEPLITZ BAND MATRICES

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Abstract. Let S(n, k) denote the $n \times n$ symmetric Toeplitz band matrix whose first k superdiagonals and first k subdiagonals have all entries 1, and whose remaining entries are all 0. For all n > k > 0 with k even, we give formulas for the nullity of S(n, k). As an application, it is shown that over

half of these matrices S(n, k) are nonsingular. For the purpose of rapid computation, we devise an algorithm that quickly computes the nullity of S(n, k) even for extremely large values of n and k, when k is even. The algorithm is based on a connection between the nullspace vectors of S(n, k) and the cycles in a certain directed graph.

Key words. Nullity, Symmetric Toeplitz band matrix, 0-1 matrix, Directed graph, Graph cycles, Multimodal.

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1 Introduction

For n > k > 0 and $x \in \mathbb{R}$, let A(n,k,x) denote the $n \times n$ skew-symmetric Toeplitz matrix whose first k superdiagonals have all entries 1, and whose remaining superdiagonal entries are all -x. For example, A(6,2,x) is the matrix

$$\begin{bmatrix} 0 & 1 & 1 & -x & -x & -x \\ -1 & 0 & 1 & 1 & -x & -x \\ -1 & -1 & 0 & 1 & 1 & -x \\ x & -1 & -1 & 0 & 1 & 1 \\ x & x & -1 & -1 & 0 & 1 \\ x & x & x & -1 & -1 & 0 \end{bmatrix}.$$

The matrices A(n, k, x) are payoff matrices for the integer choice matrix games discussed for example in [4, 5, 6]. In [3], we evaluated the nullity N(n, k) of the skew-symmetric Toeplitz band matrix A(n, k) := A(n, k, 0).

Let S(n, k) be the symmetric Toeplitz band matrix obtained from A(n, k) by removing all the minus signs, and let $N_0(n, k)$ denote the nullity of S(n, k). Theorem 3.1 yields the nontrivial periodicity result that for fixed even k, the nullity of S(n, k) equals the nullity of $S(n + (k^2 + k), k)$ for all n > k. We employ this theorem to prove our main result, Theorem 4.6, which gives a formula for the nullity of S(n, k) in terms of the known nullity N(n, k), for all n > k > 0 with k even.

In [3, Section 2], we introduced a directed graph G(n, k) on the vertices $\{0, 1, ..., k\}$ and proved that for all n > k > 0, N(n, k) equals the number of cycles in G(n, k). Call G(n, k) "parity-balanced", or for brevity "balanced",

if in each cycle, the number of even vertices equals the number of odd vertices. (This should not be confused with other meanings of balanced graphs.) In Theorem 4.7, we prove that for all n > k > 0 with k even, $N_0(n, k)$ equals the number of cycles in G(n, k) if and only if G(n, k) is balanced. We apply this theorem to create an extremely fast algorithm for computing $N_0(n, k)$. For example, Mathematica computed $N_0(1124510, 5000) = 5$ in less than .05 seconds on a basic imac. The algorithm is presented at the end of Section 4.

Price et al. [9, 10] studied the multimodality of nullity sequences of Toeplitz matrices over finite fields. This motivated our investigation in [3, Section 6], where we described the line graph connecting the points

$$(n, N(n, k)), \quad 0 \le n \le k^2 + k,$$

and showed that its shape is multimodal. In Theorem 5.1, we prove that for even k, the line graph connecting the points

$$(n, N_0(n, k)), \quad 0 \le n \le k^2 + k$$

is also multimodal. As a consequence, Corollary 5.2 shows that S(n,k) and S(n+1,k) cannot have the same nullity, unless both matrices are nonsingular. Section 5 offers several other consequences. For example, while only about 30.4% of the skew-symmetric matrices A(n,k) are nonsingular [3, Theorem 8.1], Theorem 5.7 shows that a substantially greater percentage of the symmetric matrices S(n,k) are nonsingular when k is even.

A consequence of Theorem 4.6 is that for even k,

$$(1.1) N(n,k) - N_0(n,k) \in \{0,1\}.$$

The behavior of $N_0(n,k)$ for odd k is quite different. For example, when k is odd, $N(k^2,k)=k$ and $N_0(k^2,k)=1$, so that (1.1) doesn't hold. The methods in this paper are applicable only when k is even. In hopes that the nullity $N_0(n,k)$ can be analyzed in the future for odd k, we offer number of conjectures in Section 6 to explain its behavior. For example, we conjecture a formula indicating that about 76.8% of the matrices S(n,k) are nonsingular when k is odd.

Of course S(n, k) is a very special type of Toeplitz band matrix. We refer the reader to the book [1] for properties of general Toeplitz band matrices.

2 Preliminary results and notation

Throughout this section, $k \geq 2$ is even. Lemmas 2.1–2.3 will be used in Section 3 to prove Theorem 3.1, which shows that the matrices S(n, k) and $S(n + (k^2 + k), k)$ have the same nullity.

For the roots of unity

$$\zeta_1 := \exp(2\pi i/k), \quad \zeta_2 := \exp(2\pi i/(2k+2)),$$

define the row vectors

$$u(m) := (\zeta_1^m, \zeta_1^{2m}, \dots, \zeta_1^{(k-1)m}), \quad v(m) := (\zeta_2^m, \zeta_2^{3m}, \dots, \zeta_2^{(2k+1)m}),$$

where in each vector the entry equal to $(-1)^m$ is omitted. Thus u(m) and v(m) have k-2 and k entries, respectively. Define the $k \times 1$ column vectors

$$\tau := (1, -1, 1, \dots, -1)^*, \quad s_1 := (0, 1, -2, \dots, k-1)^*,$$

where the signs alternate; here the asterisk denotes transpose. Let s_2 denote the $k \times 1$ column vector

$$s_2 = (-1)^n (s_1 - (n+k)\tau).$$

Define the $2k \times 2k$ matrix

$$V_0(n,k) := \left(\begin{array}{c|cc|c} s_1 & \tau & A & B \\ \hline s_2 & (-1)^n \tau & C & D \end{array}\right),$$

where A is the $k \times (k-2)$ matrix whose rows are $u(0), u(1), \ldots, u(k-1), B$ is the $k \times k$ matrix whose rows are $v(0), v(1), \ldots, v(k-1), C$ is the $k \times (k-2)$ matrix whose rows are $u(n+k), u(n+k+1), \ldots, u(n+2k-1)$, and D is the $k \times k$ matrix whose rows are $v(n+k), v(n+k+1), \ldots, v(n+2k-1)$. To help visualize the last 2k-2 columns, we write

$$\begin{pmatrix} u(0) & v(0) \\ \vdots & \vdots \\ u(k-1) & v(k-1) \\ \hline u(n+k) & v(n+k) \\ \vdots & \vdots \\ u(n+2k-1) & v(n+2k-1) \end{pmatrix} = \begin{pmatrix} A & B \\ \hline C & D \end{pmatrix}.$$

Note that $V_0(0, k)$ is a generalized Vandermonde matrix, so its 2k rows are independent over \mathbb{C} [7, eq. 14].

Converting the notation in [11] to ours, and noting that -1 is a double zero of the polynomial in [11, eq. (4)], we see that our matrix $V_0(n, k)$ is the $2k \times 2k$ matrix associated with S(n, k) that is defined in the top half of [11, p. 201]. Thus by [11, eq. (14)], the nullity $N_0(n, k)$ of S(n, k) equals the nullity of $V_0(n, k)$. Although the nullity of S(n, k) is only defined for n > k, we find it convenient to extend the definition of $N_0(n, k)$ so that it equals the nullity of $V_0(n, k)$ for all integers n. In particular, $N_0(0, k) = 0$.

It is not true in general that $N_0(n,k)$ equals $N_0(n+(k^2+k),k)$. For example, consider the case n=-k. The top half of $V_0(-k,k)$ is identical to the bottom half, so clearly the first column of $V_0(-k,k)$ is dependent on the other 2k-1 columns. The matrices $V_0(k^2,k)$ and $V_0(-k,k)$ are identical except for their first columns. The first column of $V_0(k^2,k)$ is clearly independent of the other 2k-1 columns. Thus for n=-k, the rank of $V_0(n,k)$ is not the same as the rank of $V_0(n+(k^2+k),k)$, i.e., $N_0(n,k)$ is not the same as $N_0(n+(k^2+k),k)$. The situation is quite different when $n \geq 0$. For nonnegative n, Theorem 3.1 shows that the first column of $V_0(n,k)$ is always independent of the other 2k-1 columns, and $N_0(n,k) = N_0(n+(k^2+k),k)$. Our proof of Theorem 3.1 depends on the lemmas below.

For $1 \le i \le k$, let e_i denote the *i*-th row or column of the $k \times k$ identity matrix I. (It will be clear from the context whether e_i is being viewed as a row vector or a column vector.) Let α denote the least nonnegative residue of n + k modulo k + 1, and let β denote the least nonnegative residue of n modulo k. Define $\epsilon = (-1)^h$, where h is the nonnegative integer satisfying $n + k = \alpha + (k + 1)h$. Since k is even, we have $\epsilon = (-1)^{n+\alpha}$ and

(2.1)
$$\beta - \alpha \equiv h \pmod{2}.$$

For each j with $0 \le j \le k - 1$,

$$v(n+k+j) = \begin{cases} \epsilon v(\alpha+j) & \text{if } \alpha+j \leq k \\ -\epsilon v(\alpha+j-k-1) & \text{if } \alpha+j \geq k+1. \end{cases}$$

Since B has rows v(j) for $0 \le j \le k-1$, it follows that $v(i)B^{-1} = e_{i+1}$ for each $0 \le i < k$. Moreover, $v(k)B^{-1} = -\tau^*$, since

$$0 = v(0) - v(1) + v(2) - \dots + v(k).$$

Since D has rows v(n+k+j) for $0 \le j \le k-1$, it follows that $\epsilon DB^{-1} = I$ when $\alpha = 0$, and otherwise ϵDB^{-1} is the matrix with rows

$$e_{\alpha+1}, \dots e_k, -\tau^*, -e_1, \dots, -e_{\alpha-1}.$$

If $\alpha = 0$, let $M := DB^{-1}$. When $\alpha > 0$, let M be the matrix obtained from DB^{-1} by replacing the $(k + 1 - \alpha)$ -th row $-\epsilon \tau^*$ by a row of zeros, so that the rows of ϵM are

$$(2.2) e_{\alpha+1}, \dots e_k, 0, -e_1, \dots, -e_{\alpha-1}.$$

Let P be the $k \times k$ permutation matrix whose rows are

$$(2.3) e_{\beta+1}, \dots e_k, e_1, \dots, e_{\beta}.$$

Observe that C = PA.

By definition of M and P, the entries in the matrix P-M all lie in $\{0,1,-1\}$, and there are at most two nonzero entries in any given row or column.

Lemma 2.1. Suppose that a given column of P - M has a pair of nonzero entries a_i and a_j in rows i and j, respectively. Then $a_i a_j = (-1)^{i+j+1}$. In other words, a_i and a_j have the same sign if and only if i and j have opposite parity. Similarly, if a given row of P - M has a pair of nonzero entries a_i and a_j in columns i and j respectively, then a_i and a_j have the same sign if and only if i and j have opposite parity.

Proof. Given a $k \times k$ matrix T, let $D_T(0)$ refer to its main diagonal, with superdiagonals $D_T(i)$ and subdiagonals $D_T(-i)$ for $1 \le i \le k-1$. Write $\omega(D_T(j)) = a$ when all entries in $D_T(j)$ are equal to a.

The nonzero entries in P are given by

$$\omega(D_P(\beta)) = 1, \quad \omega(D_P(\beta - k)) = 1,$$

and the nonzero entries in M are given by

$$\omega(D_M(\alpha)) = (-1)^h, \quad \omega(D_M(\alpha - k - 1)) = (-1)^{h+1},$$

where we ignore nonexisting diagonals $D(\pm k)$ and D(-k-1).

First suppose that h is even. Then the entries $\omega(D_{-M}(\alpha)) = -1$ and $\omega(D_P(\beta)) = 1$ have opposite signs, while the distance between the diagonal

 $D(\alpha)$ and the diagonal $D(\beta)$ or $D(\beta - k)$ is even, by (2.1). In addition, $\omega(D_{-M}(\alpha - k - 1)) = 1$ and $\omega(D_P(\beta)) = 1$ have the same sign, while the distance between the diagonal $D(\alpha - k - 1)$ and the diagonal $D(\beta)$ or $D(\beta - k)$ is odd. This proves the lemma when h is even, and the proof for odd h proceeds the same way.

Suppose that a nonzero row or column vector ν lies in the left or right nullspace of P-M. If ν no longer remains in the nullspace after a proper subset of its nonzero entries is replaced by zeros, we say that ν is *irreducible*.

Lemma 2.2. Suppose that $\nu = (\nu(1), \dots, \nu(k))$ is an irreducible vector in the left or right nullspace of P - M. Then ν can be normalized via a scalar multiple so that its nonzero entries $\nu(r)$ all satisfy $\nu(r) = (-1)^{r+1}$.

Proof. First assume that ν lies in the left nullspace of P-M. Denote the nonzero entries in ν by $\nu(r_1), \nu(r_2), \ldots, \nu(r_\ell)$. We may scale ν so that $\nu(r_1) = (-1)^{r_1+1}$. Let m be maximal such that $\nu(r) = (-1)^{r+1}$ holds for m values of r. If $m = \ell$, the proof is complete, so assume for the purpose of contradiction that $m < \ell$. Reordering the subscripts if necessary, we have

$$\nu(r_a) = (-1)^{r_a+1}, \quad a = 1, 2, \dots, m.$$

We may suppose that there exists a column Z of P-M with a nonzero entry ρ_x in row r_x for some $x \leq m$ and a nonzero entry ρ_y in row r_y for some y > m. Otherwise, replacement of ν 's entries $\nu(r_b)$ by 0 for all b > m yields a vector in the left nullspace of P-M with only m nonzero entries, contradicting the fact that ν is irreducible.

The dot product of column Z with ν equals $0 = \nu(r_x)\rho_x + \nu(r_y)\rho_y$. Since $\nu(r_x) = (-1)^{r_x+1}$, we have $\nu(r_y) = (-1)^{r_x}\rho_x/\rho_y$. By Lemma 2.1, $\rho_x/\rho_y = (-1)^{r_y-r_x+1}$. Thus $\nu(r_y) = (-1)^{r_y+1}$, contradicting the maximality of m.

Finally assume that ν is in the right nullspace of P-M. Then by mimicking the proof above using rows Z instead of columns, we complete the proof of Lemma 2.2.

When $\alpha > 0$, define a directed graph on the vertices $1, 2, \ldots, k$, with edges $x \to y$ directed from x to y if and only if for some $c \in [1, k]$, column c of P is e_x and column c of M is $\pm e_y$. By (2.2) and (2.3), the columns of P are

$$(2.4)$$
 $e_{k+1-\beta}, \ldots, e_k, e_1, \ldots, e_{k-\beta},$

and the columns of ϵM are

$$(2.5) -e_{k+2-\alpha}, \dots, -e_k, 0, e_1, \dots, e_{k-\alpha}.$$

Since no column of M can be $\pm e_{k+1-\alpha}$, the vertex $k+1-\alpha$ has in-degree 0. Letting e_d denote the α -th column of P, we see that vertex d has out-degree 0, since the α -th column of M is 0. For every other vertex, the in-degree and out-degree are both 1. Thus this digraph consists of an open path \mathcal{T} (called the "tail") together with a (possibly empty) disjoint union of simple cycles. The initial vertex of \mathcal{T} is $k+1-\alpha$ and the terminal vertex is d.

Lemma 2.3. Suppose that $\alpha > 0$. If $\nu = (\nu(1), \dots, \nu(k))$ is in the left nullspace of P - M, then $\nu(x) = 0$ for every x in the tail T. In particular, $\nu(k+1-\alpha) = 0$.

Proof. The α -th column of P-M is e_d . Thus e_d is orthogonal to ν , so that $\nu(d)=0$. We now induct back along the path \mathcal{T} , starting with the hypothesis that $x\to y$ with $\nu(y)=0$. It remains to show that $\nu(x)=0$. There is a column in P-M of the form $e_x\pm e_y$. Since this column is orthogonal to ν , we have $\nu(x)\pm\nu(y)=0$. Since $\nu(y)=0$, we conclude that $\nu(x)=0$.

3 Periodicity for the nullity of S(n,k)

Theorem 3.1. Suppose that $n \ge 0$ and k is even. Then the first column of $V_0(n,k)$ is independent of the other 2k-1 columns, and

(3.1)
$$N_0(n,k) = N_0(n + (k^2 + k), k).$$

Proof. The last 2k-1 columns of $V_0(n,k)$ are unchanged when n is replaced by $n+(k^2+k)$. Thus (3.1) is an immediate consequence of the independence of the first column. Assume for the purpose of contradiction that the first column is dependent, so that there exists a $2k \times 1$ vector $(1, a, w_1, w_2)^*$ in the nullspace of $V_0(n, k)$, where $a \in \mathbb{C}$ and where w_1 and w_2 are complex column vectors with k-2 and k entries, respectively. Since

$$w_2 = -B^{-1}Aw_1 - aB^{-1}\tau - B^{-1}s_1,$$

we have

$$(3.2) (C - DB^{-1}A)w_1 = aDB^{-1}\tau - (-1)^n a\tau + DB^{-1}s_1 - s_2.$$

First consider the case where $\alpha = 0$. Then $DB^{-1} = \epsilon I$, so that (3.2) becomes

$$(C - \epsilon A)w_1 = \epsilon s_1 - s_2 = (-1)^n (n+k)\tau.$$

Let U denote the $(k-2)\times(k-2)$ diagonal matrix diag $((\zeta_1)^{n+k},\ldots,(\zeta_1^{k-1})^{n+k})$, where the diagonal entry $(-1)^{n+k}$ is omitted. Since C=AU, we have

$$A(U - \epsilon I)w_1 = (-1)^n (n+k)\tau.$$

As n+k is nonzero, this shows that τ is a linear combination of the columns of A. But since Vandermonde matrices are invertible, τ must be independent of the columns of A, so we have our desired contradiction when $\alpha = 0$.

For the remainder of this proof, we may assume that $\alpha > 0$. Since C = PA and $\tau^*A = 0$, the left member of (3.2) equals $(P - M)Aw_1$. Since $\tau = e_1 - e_2 + \cdots - e_k$, we have

(3.3)
$$DB^{-1}\tau = (-1)^n \tau - \epsilon(k+1)e_{k+1-\alpha}.$$

Thus (3.2) becomes

$$(3.4) (P-M)Aw_1 = DB^{-1}s_1 + (-1)^{n+1}(s_1 - (n+k)\tau) - a\epsilon(k+1)e_{k+1-\alpha}.$$

We proceed to evaluate $DB^{-1}s_1$, making use of the formulas

$$s_1 = \sum_{r=1}^{k} (r-1)(-1)^r e_r, \quad \tau^* s_1 = -k(k-1)/2, \quad \epsilon = (-1)^{n+\alpha}.$$

Multiplying s_1 by each row of DB^{-1} gives

$$DB^{-1}s_{1} = \epsilon \frac{k(k-1)}{2} e_{k+1-\alpha} + (-1)^{n+1} \sum_{r=1}^{k-\alpha} (-1)^{r-1} (r+\alpha-1) e_{r}$$

$$+ (-1)^{n+1} \sum_{r=k+2-\alpha}^{k} (-1)^{r-1} (r+\alpha-k-2) e_{r}$$

$$= \epsilon \frac{k(k-1)}{2} e_{k+1-\alpha} + \alpha (-1)^{n+1} \left(\sum_{r=1}^{k-\alpha} (-1)^{r-1} e_{r} + \sum_{r=k+2-\alpha}^{k} (-1)^{r-1} e_{r} \right)$$

$$+ (-1)^{n} \left(\sum_{r=1}^{k-\alpha} (-1)^{r} (r-1) e_{r} + \sum_{r=k+2-\alpha}^{k} (-1)^{r} (r-1-k-1) e_{r} \right).$$

The sums from $k+2-\alpha$ to k are of course interpreted to be 0 if $\alpha=1$. Define

$$\tau_z := \sum_{r=z}^k (-1)^{r-1} e_r.$$

Then

$$DB^{-1}s_1 = \epsilon \frac{k(k-1)}{2} e_{k+1-\alpha} + (-1)^{n+1} \alpha \tau + \alpha (-1)^{n+\alpha} e_{k+1-\alpha} + (-1)^n \left(\left\{ s_1 + (k-\alpha)(-1)^{\alpha} e_{k+1-\alpha} \right\} + (k+1)\tau_{k+2-\alpha} \right).$$

Thus

(3.5)
$$DB^{-1}s_1 + (-1)^{n+1}s_1 = \epsilon \frac{k(k+1)}{2} e_{k+1-\alpha} + (-1)^{n+1}\alpha\tau + (k+1)(-1)^n \tau_{k+2-\alpha}.$$

Together with (3.4), this yields

(3.6)
$$(P - M)Aw_1 = (-1)^n (n + k - \alpha)\tau$$

$$+ (-1)^n (k+1)\tau_{k+2-\alpha} + \left(\epsilon \frac{k(k+1)}{2} - a\epsilon (k+1)\right) e_{k+1-\alpha}.$$

We now consider separately the cases where P-M is singular and where P-M is nonsingular. First consider the singular case. In this case n>0, because when n=0, we have $\alpha=k$ and $\beta=0$, so that P-M is the nonsingular lower triangular matrix with 1's along the main diagonal and the first subdiagonal. Let ν be the left nullspace vector in Lemma 2.2. After left-multiplying both sides of (3.6) by ν , that equation reduces to

(3.7)
$$0 = (n+k-\alpha)\nu\tau + (k+1)\nu\tau_{k+2-\alpha},$$

because $\nu e_{k+1-\alpha} = 0$ by Lemma 2.3. By Lemma 2.2, $\nu \tau = \ell$, where $\ell > 0$ is the number of nonzero entries in ν . Moreover, $\nu \tau_{k+2-\alpha} \geq 0$. Thus, since n > 0, the right member of (3.7) is positive, which gives the desired contradiction.

It remains to consider the case where P-M is invertible. We begin by showing that

(3.8)
$$\sigma(P-M)^{-1}e_{k+1-\alpha} = 0,$$

where σ is the $1 \times k$ row vector whose entries are all 1. It follows from (3.3) that

$$M\tau = (-1)^n \tau - \epsilon e_{k+1-\alpha}.$$

Since $P\tau = (-1)^{\beta}\tau$, we see that

$$(P-M)\tau = \epsilon e_{k+1-\alpha} + \tau \left((-1)^{\beta} - (-1)^n \right).$$

The rightmost term vanishes since β and n have the same parity. Thus $\tau = \epsilon (P - M)^{-1} e_{k+1-\alpha}$, and (3.8) follows since $\sigma \tau = 0$.

After left-multiplying (3.6) by $\sigma(P-M)^{-1}$, the left member reduces to 0, because $\sigma A=0$. Thus (3.6) reduces to

(3.9)
$$0 = \sigma(P - M)^{-1} \left((n + k - \alpha)\tau + (k+1)\tau_{k+2-\alpha} \right),$$

in view of (3.8).

Using the formula $-\tau^* s_1 = k(k-1)/2$, we deduce from (3.5) that

$$(-1)^n M s_1 \equiv s_1 - \alpha \tau + (k+1) \tau_{k+2-\alpha} \pmod{k}.$$

Subtract $(-1)^n Ps_1$ to get

$$(-1)^n (M-P) s_1 \equiv (I - (-1)^n P) s_1 - \alpha \tau + (k+1) \tau_{k+2-\alpha} \pmod{k}.$$

It follows from the definitions of P, s_1 , and β that

$$(I - (-1)^n P) s_1 \equiv \beta \tau \equiv n\tau \pmod{k}.$$

Combine the last two congruences to obtain

$$(-1)^n (M-P) s_1 \equiv (n+k-\alpha)\tau + (k+1)\tau_{k+2-\alpha} \pmod{k}.$$

Left-multiplying by $(P-M)^{-1}$, we obtain

$$-(-1)^n s_1 \equiv (P - M)^{-1} \left((n + k - \alpha)\tau + (k+1)\tau_{k+2-\alpha} \right) \pmod{k}.$$

Left-multiplication by σ yields

$$(-1)^{n}k/2 \equiv \sigma(P-M)^{-1} ((n+k-\alpha)\tau + (k+1)\tau_{k+2-\alpha}) \pmod{k}.$$

The right member above is therefore an odd multiple of k/2, so it cannot vanish. This contradicts (3.9).

4 The nullity of S(n,k)

Throughout this section, $k \geq 2$ is even. In Lemma 4.4 we show that the nullity of the $k \times k$ matrix H := M - P equals N(n,k) (which in turn is evaluated in [3]). Let \overline{H} be the $(k+1) \times k$ matrix obtained from H by appending the row $\sigma = (1,1,\ldots,1)$. Theorem 4.6 shows that the nullity $N_0(n,k)$ of S(n,k) equals $k - \operatorname{rank}\overline{H}$. Consequently, $N_0(n,k) = N(n,k)$ when σ is in the row space of H, and $N_0(n,k) = N(n,k) - 1$ otherwise. The proofs depend on another directed graph which we call $G_0(n,k)$. The vertices of $G_0(n,k)$ are $1,2,\ldots,k$, with edges $a \to b$ directed from a to b if and only if for some $r \in [1,k]$, row r of M is $\pm e_a$ and row r of P is e_b .

Let $(x)_{k+1}$ and $(x)_k$ denote the least nonnegative residues of x modulo k+1 and k, respectively. If $\alpha > 0$, then $G_0(n,k)$ has the k-1 edges

$$(a+n-1)_{k+1} \to 1 + (a+n-1)_k, \quad a \in [1,k], \qquad a \neq (k+1-\alpha).$$

In this case, the graph is a union of disjoint cycles together with a tail whose initial vertex is $1 + (\beta - \alpha)_k$ and whose terminal vertex is α . (If it happens that the initial and terminal vertices coincide, then the tail consists of the isolated vertex α .) If $\alpha = 0$, then $G_0(n, k)$ has the k edges

$$(a+n-1)_{k+1} \to 1 + (a+n-1)_k, \quad a \in [1, k].$$

In this case, the graph is a union of disjoint cycles with no tail.

The digraph $G_0(n, k)$ is very similar to the digraph G(n, k), which was analyzed in [3]. Indeed, after one discards the vertex k from the tail of G(n, k) (should k appear), we see from [3, eq. (2.2)] that the edges of $G_0(n, k)$ are simply translates by +1 of the edges of G(n, k). For example, G(26, 10) has the two cycles

$$0 \rightarrow 4 \rightarrow 7 \rightarrow 0$$
, $1 \rightarrow 5 \rightarrow 8 \rightarrow 1$

and the tail $10 \to 3 \to 6 \to 9 \to 2$, while $G_0(26, 10)$ has the two cycles

$$1 \rightarrow 5 \rightarrow 8 \rightarrow 1$$
, $2 \rightarrow 6 \rightarrow 9 \rightarrow 2$

and the tail $4 \to 7 \to 10 \to 3$. In view of what has been proved about G(n, k) in [3], it follows that for a given pair $n, k, G_0(n, k)$ has exactly N(n, k) disjoint cycles, all translates of each other, hence all of the same length.

Let $\mathcal{N}(H)$ denote the (right) nullspace of H. The following lemma is analogous to Lemma 2.3.

Lemma 4.1. If $\nu = (\nu(1), \dots, \nu(k))$ is a column vector in $\mathcal{N}(H)$, then $\nu(x) = 0$ for every x in the tail of $G_0(n, k)$.

Proof. Let c denote the initial vertex in the tail (so $\alpha > 0$). Since row $k+1-\alpha$ of H is $-e_c$ and this row is orthogonal to ν , we have $\nu(c) = 0$. Now induct along the tail. Assuming that $x \to y$ and $\nu(x) = 0$, we must show that $\nu(y) = 0$. Some row of H is $\pm e_x - e_y$, so $\nu(y) = \pm \nu(x) = 0$, as desired. \square

Let $\mathcal{S} \subset [1,k]$. If \mathcal{S} is the set of vertices in a cycle \mathcal{C} in $G_0(n,k)$, we say that \mathcal{C} is an \mathcal{S} -cycle. If the set of nonzero entries in a column vector $\nu = (\nu(1), \dots, \nu(k))$ is $\{\nu(x) = (-1)^{x+1} : x \in \mathcal{S}\}$, we say that ν is an \mathcal{S} -vector.

Lemma 4.2. Let C be an S-cycle in $G_0(n, k)$, and let ν be an S-vector. Then $\nu \in \mathcal{N}(H)$.

Proof. For every row μ of H, we will show that $\mu\nu = 0$. If μ has only one nonzero entry, then $\mu = -e_c$ where c is the initial vertex in the tail of $G_0(n,k)$. By Lemma 4.1, $\nu(c) = 0$, so that $\mu\nu = 0$. Thus we may suppose that $\mu = \pm e_a - e_b$, where $\pm e_a$ comes from M and e_b comes from P. More precisely, by Lemma 2.1, $\mu = (-1)^{a+b}e_a - e_b$. By definition, $G_0(n,k)$ has the edge $a \to b$. If this edge is not part of the cycle \mathcal{C} , then $\nu(a) = \nu(b) = 0$ by definition of ν , so that $\mu\nu = 0$. If the edge is part of \mathcal{C} , then

$$\mu\nu = (-1)^{a+b}(-1)^{a+1} - (-1)^{b+1} = 0.$$

Thus $\mu\nu = 0$ in all cases.

Lemma 4.3. Let ν be an irreducible S-vector in $\mathcal{N}(H)$. Then $G_0(n,k)$ has an S-cycle.

Proof. Since $\nu(x)$ is nonzero for all $x \in \mathcal{S}$, no $x \in \mathcal{S}$ can be in the tail of $G_0(n,k)$, i.e., every $x \in \mathcal{S}$ is in some cycle. Thus some cycle \mathcal{C} in $G_0(n,k)$ has an edge of the form $a \to b$ with $a \in \mathcal{S}$. Therefore H has a row $\mu = (-1)^{a+b}e_a - e_b$. Since $\nu \in \mathcal{N}(H)$, we have $(-1)^{a+b}(-1)^{a+1} - \nu(b) = 0$, which forces $\nu(b) = (-1)^{b+1}$. Thus $b \in \mathcal{S}$. Repeating this argument with b in place of a, and so on, we see that the vertices in cycle \mathcal{C} must lie in a subset $\mathcal{S}' \subset \mathcal{S}$. If \mathcal{S}' were a proper subset of \mathcal{S} , then by Lemma 4.2, an \mathcal{S}' -vector would lie in $\mathcal{N}(H)$, contradicting the fact the ν is irreducible. Thus \mathcal{C} is the desired \mathcal{S} -cycle.

The vector ν in Lemma 4.2 must be irreducible in $\mathcal{N}(H)$. Otherwise there would exist an \mathcal{S}' -vector in $\mathcal{N}(H)$ for some proper subset \mathcal{S}' of \mathcal{S} . But then by Lemma 4.3, $G_0(n,k)$ would have an \mathcal{S}' -cycle in addition to the \mathcal{S} cycle \mathcal{C} . This is impossible, since all cycles in $G_0(n,k)$ have the same length. It is now clear that Lemmas 4.2–4.3 together show that there is a one-toone correspondence between cycles in $G_0(n,k)$ and normalized irreducible vectors in $\mathcal{N}(H)$. (Here "normalized" is meant in the sense of Lemma 2.2.) The correspondence associates an \mathcal{S} -cycle in $G_0(n,k)$ with an irreducible \mathcal{S} -vector in $\mathcal{N}(H)$.

Lemma 4.4. The dimension of $\mathcal{N}(H)$ is N(n,k).

Proof. Let C_1, \ldots, C_N denote the N = N(n, k) cycles in $G_0(n, k)$. Let S_i be the set of vertices in C_i , for each i. To each C_i there corresponds an irreducible S_i -vector v_i in $\mathcal{N}(H)$. Every vector in $\mathcal{N}(H)$ is a sum of irreducible vectors. Thus the normalized irreducible vectors in $\mathcal{N}(H)$ generate $\mathcal{N}(H)$. By Lemma 4.3, the v_i are the only normalized irreducible vectors in $\mathcal{N}(H)$. Thus v_1, \ldots, v_N generate $\mathcal{N}(H)$. Moreover, v_1, \ldots, v_N is a basis for $\mathcal{N}(H)$, since the S_i are disjoint. Thus $\mathcal{N}(H)$ has dimension N.

Recall that H := M - P. Define the related matrix $J := DB^{-1} - P$. Analogous to our definition of \overline{H} , let \overline{J} be the $(k+1) \times k$ matrix obtained from J by appending the row $\sigma = (1, 1, ..., 1)$.

Lemma 4.5. We have $\operatorname{rank}(J) = \operatorname{rank}(H)$ and $\operatorname{rank}(\overline{J}) = \operatorname{rank}(\overline{H})$.

Proof. If $\alpha = 0$, the result is obvious since J = H, so assume that $\alpha > 0$. The $(k+1-\alpha)$ -th row of H is $-e_c$ for some c, and the $(k+1-\alpha)$ -th row of J is $-\epsilon\tau^* - e_c$. The other k-1 rows H and J are the same. Let \mathcal{R} denote the row space of these k-1 rows. By Lemma 2.1, the inner product $\rho\tau$ vanishes for every $\rho \in \mathcal{R}$. To prove that $\operatorname{rank}(J) = \operatorname{rank}(H)$, it suffices to show that neither e_c nor $\epsilon\tau^* + e_c$ lies in \mathcal{R} . This follows because

$$e_c \tau = \pm 1 \neq 0$$
, $(\epsilon \tau^* + e_c) \tau = \epsilon k \pm 1 \neq 0$.

To prove $\operatorname{rank}(\overline{J}) = \operatorname{rank}(\overline{H})$, it suffices to prove that $\sigma \in \mathcal{R}$ whenever σ is in the row space of either H or J. If $\sigma = \rho + re_c$ for some $\rho \in \mathcal{R}$ and some real r, then since $\sigma \tau = 0 = \rho \tau$, we have r = 0, so that $\sigma = \rho \in \mathcal{R}$. Finally, if $\sigma = \rho + r(\epsilon \tau^* + e_c)$ for some $\rho \in \mathcal{R}$ and some real r, then since $\sigma \tau = 0 = \rho \tau$, we have $r(\epsilon k \pm 1) = 0$, so that r = 0 and $\sigma = \rho \in \mathcal{R}$.

We are finally in a position to evaluate the nullity $N_0(n,k)$ of the matrix S(n,k) for even k.

Theorem 4.6. For even k, $N_0(n,k) = k-\text{rank}(\overline{H})$. Equivalently, $N_0(n,k) = N(n,k)$ when σ is in the row space of H, and $N_0(n,k) = N(n,k) - 1$ otherwise.

Proof. Let V be the $2k \times 2k$ matrix obtained from $V_0(n,k)$ by replacing the first column by the zero column. By Theorem 3.1, the first column of $V_0(n,k)$ is independent of its other columns, so that $\operatorname{rank}(V_0(n,k)) = 1 + \operatorname{rank}(V)$. We write

$$V := \left(\begin{array}{c|c} A' & B \\ \hline PA' & D \end{array}\right),$$

where A', B, PA', D are $k \times k$ matrices. Here B and D are the same matrices that appeared in the definition of $V_0(n, k)$. Because row operations preserve rank, we have rank(V) = rank(V_1), where

$$V_1 := \left(\begin{array}{c|c} A' & B \\ \hline 0 & D - PB \end{array}\right).$$

Multiplying V_1 on the right by

$$\left(\begin{array}{c|c} I & 0 \\ \hline 0 & B^{-1} \end{array}\right),\,$$

we obtain the matrix

$$V_2 = \left(\begin{array}{c|c} A' & I \\ \hline 0 & J \end{array}\right),$$

where we recall that $J := DB^{-1} - P$. The ranks of V, V_1 , and V_2 are all equal to $\operatorname{rank}(V_0(n,k)) - 1$.

The span of the top k rows of V_2 has dimension k, and the span of the bottom k rows has dimension $\operatorname{rank}(J)$. Thus $\operatorname{rank}(V_2) \leq k + \operatorname{rank}(J)$. On the other hand, $\operatorname{rank}(V_2) \geq k - 1 + \operatorname{rank}(J)$, with equality if and only if σ is in the row space of J. This is because the k column sums of A' all vanish, and up to scalar multiple, the sum of the top k rows of V_2 is the only linear combination of these k rows that can lie in the span of the bottom k rows. Consequently, $\operatorname{rank}(V_2) = k - 1 + \operatorname{rank}(\overline{J})$, so that

$$rank(V_0(n, k)) = k + rank(\overline{J}) = k + rank(\overline{H}),$$

where the last equality follows from Lemma 4.5. Thus the nullity $N_0(n, k)$ of $V_0(n, k)$ is $k - \text{rank}(\overline{H})$. Finally, the last statement in Theorem 4.6 follows because k - rank(H) = N(n, k) by Lemma 4.4.

The digraph G(n,k) will be called "balanced" if in each cycle, the number of even vertices equals the number of odd vertices. For example, G(28,12) is balanced because its cycle $1 \to 4 \to 7 \to 10 \to 1$ (and its translate) has two odd vertices and two even vertices. For another example, G(22,12) is balanced because it has no cycles. Note that G(n,k) is necessarily unbalanced if it has a cycle of odd length.

Theorem 4.7. If G(n,k) is balanced, then $N_0(n,k) = N(n,k)$; otherwise $N_0(n,k) = N(n,k) - 1$.

Proof. The row space of H is equal to $\mathcal{N}(H)^{\perp}$. Let the \mathcal{S}_i -cycle \mathcal{C}_i and the \mathcal{S}_i -vector ν_i be as in the proof of Lemma 4.4. We have $\sigma \in \mathcal{N}(H)^{\perp}$ if and only if for each i,

$$\sigma \nu_i = \sum_{x \in \mathcal{S}_i} (-1)^{x+1} = 0.$$

Thus $\sigma \in \mathcal{N}(H)^{\perp}$ if and only if G(n,k) is balanced. The result now follows from Theorem 4.6.

In view of Theorem 4.6, we could compute the rank of \overline{H} in order to determine whether the nullity of S(n,k) is N(n,k) or N(n,k)-1. However, if k is very large, such a time-consuming computation would be impractical. In contrast, the following Mathematica function based on Theorem 4.7 quickly computes the nullity of S(n,k) for extremely large values of n and k with k even.

5 Line graph connecting points $(n, N_0(n, k))$

Fix k with k even. The line graph connecting successive Cartesian points $(n, N_0(n, k))$ for $n \geq 0$ will be called a G_0 -graph, while the line graph in [3] connecting the points (n, N(n, k)) for $n \geq 0$ will be called a G-graph. By (3.1), for $n \geq 0$, the nullity $N_0(n, k)$ depends only on the value of n modulo $(k^2 + k)$, so we can restrict our G_0 -graph to values of n between 0 and $(k^2 + k)$. For k = 6, $0 \leq n \leq 42$, the G_0 -graph is illustrated by the solid line in Figure 1, and the G-graph is illustrated by the dashed line. Each dot on the horizontal axis in Figure 1 indicates a point where $N_0(n, k) = 0$. For example, the dot at the point (19,0) indicates that the matrix S(19,6) is nonsingular.

In [3, Section 6], we proved that the G-graph is multimodal by showing that the union of the horizontal axis with the G-graph has the shape of a chain of adjoining isosceles right triangles whose hypotenuses sit on the horizontal axis. Theorem 5.1 shows that the union of the G_0 -graph with the horizontal axis also has the shape of a chain of isosceles right triangles, so that the G_0 -graph is also multimodal. However, unlike the G-graph, the G_0 -graph has many triangles that are not adjoining.

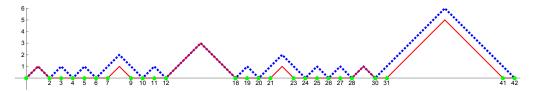


Figure 1: Line graph for k = 6

An apex (n, N(n, k)) of a right triangle in the G-graph for which G(n, k) is balanced will be called a balanced apex, and the triangle to which it belongs will be called a balanced triangle. For example, the balanced triangles in Figure 1 are the ones with apexes (1, 1), (15, 3), and (29, 1). As we descend from a balanced apex (n, N(n, k)) to any point (n', N(n', k)) above the horizontal axis lying on the same triangle, the corresponding digraph G(n', k) remains balanced, because by [3, Section 6], it must have a cycle in common with G(n, k). For example, descending from the balanced apex (15, 3) in Figure 1, we see that the digraphs G(n, 6) for n = 13, 14, 15, 16, 17 are balanced because each has a cycle in common with G(15, 6).

The shape of the G_0 -graph is best described by comparing it with the

well-understood G-graph. We continue to use Figure 1 as a running example. By Theorem 4.7, $N_0(n,k) = N(n,k)$ for every point (n,N(n,k)) on a balanced triangle. Thus the G_0 -graph will have a triangle coincident with each balanced triangle in the G-graph. For Figure 1, this explains why the solid and dashed triangles with apexes (1,1), (15,3), and (29,1) are coincident.

Next consider the unbalanced triangles in the G-graph with height greater than 1. In Figure 1, these are the triangles with apexes (8,2), (22,2), and (36,6). As we descend from an unbalanced apex (n, N(n, k)) along either leg of the triangle, the corresponding digraphs remain unbalanced, until we reach points on the horizontal axis, for which the corresponding digraphs have no cycles. By Theorem 4.7, $N_0(n, k) = N(n, k) - 1$ for every point (n, N(n, k)) on an unbalanced triangle, except when N(n, k) = 0. Thus the G_0 -graph will have a triangle lying one unit below each unbalanced triangle in the G-graph with height greater than 1. For Figure 1, this explains why the solid triangles lie one unit below the dashed triangles with apexes (8, 2), (22, 2), and (36, 6).

Finally, consider the unbalanced triangles in the G-graph which have height 1. In Figure 1, these are the triangles with apexes (3,1), (5,1), (11,1), (19,1), (25,1), and (27,1). The portion of the G_0 -graph lying underneath an unbalanced triangle of height 1 must reduce to a degenerate triangle lying on the horizontal axis. For Figure 1, this explains why the hypotenuse belonging to each of the dashed triangles with apexes (3,1), (5,1), (11,1), (19,1), (25,1), (27,1) coincides with a solid line from the G_0 -graph.

We have now proved the following theorem.

Theorem 5.1. The union of the G_0 -graph with the horizontal axis has the shape of a chain of isosceles right triangles whose hypotenuses sit on the horizontal axis. In particular, the G_0 -graph is multimodal.

Corollary 5.2. Let k be even. The nullities of S(n,k) and S(n+1,k) differ by exactly 1 unless both matrices are nonsingular.

Proof. Assume that least one of the two matrices is singular. Then the result follows from Theorem 5.1, since the two points $(n + 1, N_0(n + 1, k))$ and $(n, N_0(n, k))$ on the G_0 -graph are neighboring points on a leg of a non-degenerate right triangle.

The next theorem gives the height for a class of balanced triangles. Of course, once the height of a triangle is known, we know the nullity $N_0(n, k)$

at every other point in that triangle. For example, Theorem 5.3 shows that if n = 2k + 3 and $3 \mid k$, then $N_0(n, k) = 3$, $N_0(n \pm 1, k) = 2$, $N_0(n \pm 2, k) = 1$, and $N_0(n \pm 3, k) = 0$.

Theorem 5.3. Let k be even and suppose that n = (c-1)k + c for some odd c with 1 < c < k. Let $f = \gcd(c, k)$. Then S(n, k) has nullity f and the point (n, f) is a balanced apex on the G-graph.

Proof. By the proof of [3, Theorem 8.8], the digraph G(n, k) is the union of f disjoint cycles (with no tail), and the point (n, f) is an apex on the G-graph. In particular, N(n, k) = f. It remains to prove that $N_0(n, k) = f$.

Let \mathcal{C} denote the cycle in G(n, k) containing the vertex 0. The remaining cycles are contiguous translates of \mathcal{C} , by [3, Theorem 3.9]. Since f is odd, the remaining cycles can be paired off as

$$(C+2i-1) \cup (C+2i), \quad 1 \le i \le (f-1)/2.$$

Each of these (f-1)/2 disjoint unions has the same number of odd vertices as even vertices. Thus the same is true about \mathcal{C} , since the set of vertices in all f cycles is $\{0, 1, 2, \ldots, k-1\}$. Therefore G(n, k) is balanced, and the result follows from Theorem 4.7.

The next theorem gives the height for a class of unbalanced triangles.

Theorem 5.4. For k even, let t be a positive integer such that (t+1) divides (k+1). Then S(tk,k) has nullity t-1 and the point (tk,t) is an unbalanced apex on the G-graph. In particular, $S(k^2,k)$ has nullity k-1.

Proof. By [3, Theorem 8.7], the point (tk, t) is an apex in the G-graph, N(tk, k) = t, and G(tk, k) has cycles of length q := (k+1)/(t+1). Since q is odd, G(tk, k) is necessarily unbalanced. Thus by Theorem 4.7,

$$N_0(tk, k) = N(tk, k) - 1 = t - 1.$$

This completes the proof.

We remark that by [3, Theorem 7.5], the G-graph attains its maximum height k at only one apex, namely at the unbalanced apex (k^2, k) . Thus the G_0 -graph attains its maximum height k-1 at its apex $(k^2, k-1)$. Moreover, for k > 2, this is the only apex in the G_0 -graph of height k-1. To see this, assume the contrary. Then there would exist a balanced apex in the G-graph of height k-1. Applying the formula [3, eq.(7.11)] with the height f = k-1, we see that no cycle length q exists for which k-1 = f = [k/q].

Theorem 5.5. The nullity of $S((k^2-k)/2, k)$ equals k/2-1 or k/2 according as k/2 is even or odd.

Proof. By [3, Theorem 8.10] with a=0, b=2, the digraph $G((k^2-k)/2, k)$ has f=k/2 cycles each of length q=2. Thus $N((k^2-k)/2, k)=f=k/2$. By Theorem 4.7, it remains to show that $G((k^2-k)/2, k)$ is balanced if and only if k/2 is odd. By [3, eqs. (7.15-7.16)], this digraph has a cycle whose two vertices are c(0)=k/2 and c(1)=0. This digraph is balanced if and only if k/2 is odd.

For even k, let B(k) denote the number of balanced triangles in the G-graph. For k = 5000, B(k) = 75920, which gives $B(k)/k^2 \simeq .003$. This and similar data suggests to us that for large k, the balanced triangles may be relatively rare, so we propound the following conjecture.

Conjecture 5.6. As $k \to \infty$, $B(k)/k^2$ approaches 0.

For any fixed nonnegative integer z and even k, let $Q_z(k)$ denote the percentage of matrices S(n,k) with $n \in [k+1,k^2+2k]$ for which S(n,k) has nullity z. (Equivalently, $Q_z(k)$ is the percentage of $n \in [0,k^2+k)$ for which $N_0(n,k)=z$.) Theorem 5.7 shows that more than 55.7% of the matrices S(n,k) are nonsingular, and in fact, more than 68.3% of the matrices S(n,k) are nonsingular if Conjecture 5.6 holds. For $z \geq 1$, Theorem 5.8 provides asymptotic formulas for $Q_z(k)$ as $k \to \infty$, conditional on Conjecture 5.6. The proofs employ the well-known asymptotic formulas [8, Lemma 2]

$$\sum_{q \le x} \phi(x) \sim \frac{3x^2}{\pi^2}, \quad \sum_{q \le x, \ 2 \nmid q} \phi(x) \sim \frac{2x^2}{\pi^2},$$

where ϕ is the Euler totient function.

Theorem 5.7. For large even k, $Q_0(k) > 55.7\%$. In fact, if Conjecture 5.6 holds,

$$Q_0(k) \sim 6.75/\pi^2 \simeq 68.4\%, \quad as \ k \to \infty.$$

Proof. To evaluate $Q_0(k)$, we must count the number Γ of points on the G_0 -graph that lie on the horizontal axis. Write $\Gamma = \Gamma_1 + \Gamma_2$, where Γ_1 counts only the subset of points that lie on the G-graph. Each unbalanced triangle of height > 1 contributes 2 to Γ_2 , while each unbalanced triangle of height 1 contributes only 1 to Γ_2 . (For example, in Figure 1, the contributions for

height 1 come from the points 3, 5, 11, 19, 25, 27, and the contributions for height > 1 come from the pairs $\{7, 9\}, \{21, 23\}, \{31, 41\}$.) Arguing as in the proof of [3, Theorem 8.2], we see that

$$\Gamma_2 \ge \sum_{q \le k, \ 2 \nmid q} \phi(q) + \sum_{q \le k/2, \ 2 \nmid q} \phi(q).$$

Here we have taken the sums only over odd q, because cycles of even length q are not necessarily unbalanced. As in the proof of [3, Theorem 8.1],

$$\Gamma_1 = \sum_{q \le k} \phi(q).$$

Thus Γ/k^2 is greater or equal to an expression which is asymptotic to

$$(3+2+1/2)/\pi^2 = 5.5/\pi^2 \simeq .5572$$
, as $k \to \infty$.

Now suppose that Conjecture 5.6 holds. Then the balanced triangles are negligible for our purposes, so we can remove the restrictions $2 \nmid q$ on the sums above to conclude that

$$\Gamma/k^2 \sim (3+3+3/4)/\pi^2 = 6.75/\pi^2 \simeq .684$$
, as $k \to \infty$.

This completes the proof.

For k=5000, the exact number of nonsingular matrices S(n,k) with $n \in [k+1,k^2+2k]$ is 17007988. Note that 17007988/5000² $\simeq 68.0\%$, which is not far from the conditional estimate 68.4% given for large k in Theorem 5.7.

Theorem 5.8. Let k be even, and fix an integer $z \ge 1$. Assume that Conjecture 5.6 holds. Then

$$Q_z(k) \to 3(1/(z+1)^2 + 1/(z+2)^2)/\pi^2$$
, as $k \to \infty$.

Proof. Since the balanced triangles are assumed to be negligible, the proof for the G_0 -graph proceeds exactly as in the proof for the G-graph in [3, Theorem 8.2], except with z + 1 in place of z.

For k=1000, the number of S(n,k) of nullity 1 with $n \in [k+1, k^2+2k]$ is 114552. Note that $114552/1000^2 \simeq 11.4\%$, not far from the conditional estimate $13/(12\pi^2) \simeq 11.0\%$ given for $Q_1(k)$ in Theorem 5.8.

6 Conjectures for odd k

A vector (x_1, \ldots, x_n) is said to be symmetric if $(x_1, \ldots, x_n) = (x_n, \ldots, x_1)$, and it is said to be skew-symmetric if $(x_1, \ldots, x_n) = -(x_n, \ldots, x_1)$. By [2, Theorem 8], the nullspace of S(n, k) has an orthogonal basis consisting of δ symmetric vectors and θ skew-symmetric vectors, where $|\delta - \theta| \leq 1$. In particular, if $N_0(n, k) = 1$, then the nullspace of S(n, k) is generated by a vector which is either symmetric or skew-symmetric. We don't know a simple way to predict the values of n that distinguish between these two possibilities, but rather complicated determinant criteria are given near the end of Trench's Lecture Notes in [12]. Note that in Trench's determinant formulas, +1 should be corrected to -1.

When k is odd, the $2k \times 2k$ matrix associated with S(n, k) in [11, p. 201] has entries which are all powers of $\exp(2\pi i/k)$ or $\exp(2\pi i/(2k+2))$, and in contrast with the situation for even k, the polynomial in [11, eq.(4)] has distinct zeros. Thus we see that for fixed odd k, $N_0(n, k)$ has period $2k^2 + 2k$, twice the period given in (3.1) for even k.

From now on, let k be odd. For any fixed integer $z \ge 0$, let $W_z(k)$ denote the number of $n \in [0, 2k^2 + 2k)$ for which $N_0(n, k) = z$. When z = 1, we have

$$W_1(k) = W_1'(k) + W_1''(k),$$

where $W'_1(k)$ (resp. $W''_1(k)$) counts those $n \in [0, 2k^2 + 2k)$ for which the nullspace of S(n, k) is generated by a symmetric (resp. skew-symmetric) vector.

Substantial computer evidence suggests that the behavior of the nullity $N_0(n, k)$ for odd k is explained by the following conjectures.

Conjecture 6.1. Theorem 5.1 (which was stated for even k) also holds for odd k.

Conjecture 6.2. $W'_1(k)$ equals the number of $n \in [0, k^2+k)$ for which S(n, k) and $S(n + (k^2 + k), k)$ are both singular.

Conjecture 6.3. $W_1'(k)/k^2 \to 0$ as $k \to \infty$.

Conjecture 6.4. $N_0(n, k) = 0$ if (but not only if) the digraph G(n, k) has a cycle of even length.

Conjecture 6.5. $N_0(n, k) \in \{N(n, k), 0, 1\}$. Specifically, if $N_0(n, k) > 1$, then $N_0(n, k) = N(n, k)$, and if $N_0(n, k) = 1$, then n is odd and $N_0(n, k) \leq 1$

N(n,k) with equality if (but not only if) the nullspace of S(n,k) is generated by a skew-symmetric vector.

Conjecture 6.6.

$$W_1(k) = W_1'(k) + \sum_{q \le k, \ 2 \nmid q} \phi(q) + \sum_{q \le k/2, \ 2 \nmid q} \phi(q),$$

and for $z \geq 2$,

$$W_z(k) = \sum_{q \leq k/z, \ 2 \nmid q} \phi(q) \quad + \sum_{q \leq k/(z+1), \ 2 \nmid q} \phi(q).$$

For $z \geq 2$, Conjecture 6.6 gives the conditional result that the percentage of matrices S(n,k) with nullity z equals $(z^{-2} + (z+1)^{-2})/\pi^2$. For z=1, Conjectures 6.6 and 6.3 give the conditional result that the percentage of matrices S(n,k) with nullity 1 equals $1.25/\pi^2 \simeq 12.7\%$. For k=501, exactly 68287 matrices S(n,k) with $n \in [0,2k^2+2k)$ have nullity 1. Note that $68287/(2*501^2) \simeq 13.6\%$, not far from the conditional estimate 12.7% for large k.

By definition of $W_z(k)$,

$$W_0(k) = 2k^2 + 2k - \sum_{z=1}^{k} W_z(k).$$

Thus by Conjecture 6.6,

$$W_0(k) = 2k^2 + 2k - W_1'(k) + \sum_{q \le k, \ 2 \nmid q} \phi(q) - 2\sum_{z=1}^k \sum_{q \le k/z, \ 2 \nmid q} \phi(q).$$

Together with Conjecture 6.3, this gives the conditional result that the percentage of nonsingular matrices S(n,k) equals

$$1 + 0 + 1/\pi^2 - 1/3 = 2/3 + 1/\pi^2 \simeq 76.8\%.$$

For k = 501, exactly 381622 matrices S(n, k) with $n \in [0, 2k^2 + 2k)$ are non-singular. Note that $381622/(2*501^2) \simeq 76.0\%$, not far from the conditional estimate 76.8% for large k.

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