On eigenvalues of Seidel matrices and Haemers' conjecture

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Dedicated to Andries E. Brouwer on the occasion of his 65th birthday.

Abstract

For a graph G, let $S(G)$ be the Seidel matrix of G and $\theta_1(G),\dots,\theta_n(G)$ be the eigenvalues of $S(G)$. The Seidel energy of G is defined as $|\theta_1(G)|+\cdots+|\theta_n(G)|$. Willem Haemers conjectured that the Seidel energy of any graph with n vertices is at least $2n-2$, the Seidel energy of the complete graph with n vertices. Motivated by this conjecture, we prove that for any α with $0<\alpha<2$, $|\theta_1(G)|^\alpha+\cdots+|\theta_n(G)|^\alpha \geqslant (n-1)^\alpha+n-1$ if and only if $|\det S(G)|\geqslant n-1$. This, in particular, implies the Haemers' conjecture for all graphs G with $|\det S(G)|\geqslant n-1$. A computation on the fraction of graphs with $|\det S(G)|<n-1$ is reported. Motivated by that, we conjecture that almost all graphs G of order n satisfy $|\det S(G)|\geqslant n-1$. In connection with this conjecture, we note that almost all graphs of order n have a Seidel energy of $\Theta(n^{3/2})$. Finally, we prove that self-complementary graphs G of order $n\equiv 1 \pmod 4$ have $\det S(G)=0$.

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1 Introduction

Let G be a simple graph with vertex set $\{v_1, \ldots, v_n\}$. The *Seidel matrix* of G is an $n \times n$ matrix $S = S(G)$ where $S_{11} = \cdots = S_{nn} = 0$ and for $i \neq j$, S_{ij} is -1 if v_i and v_j are adjacent, and is 1 otherwise. The *adjacency matrix* of G denoted by $A = A(G)$ is defined similarly by $A_{ij} = 1$ if v_i and v_j are adjacent, and $A_{ij} = 0$ otherwise. Clearly, $S(G) = A(\overline{G}) - A(G)$ where $\overline{G}$ denotes the complement of G. The *Seidel energy* of G, denoted by $\mathcal{S}(G)$, is defined as the sum of the absolute values of the eigenvalues of $S(G)$.

Considering the complete graph K_n, its Seidel matrix is $I - J$. Hence the eigenvalues of $S(K_n)$ are $1-n$ and 1 (the latter with multiplicity $n-1$). So $\mathcal{S}(K_n) = 2n-2$. Haemers conjectured that this is the smallest Seidel energy of an n-vertex graph:

Conjecture (Haemers [6]). *For any graph G on n vertices, $\mathcal{S}(G) \geqslant \mathcal{S}(K_n)$.*

We show that the conjecture is true if $|\det S(G)| \geqslant |\det S(K_n)| = n - 1$. To be more precise, we prove the following more general statement which makes the main result of the present paper.

Theorem 1. *Let G be a graph with n vertices and let $\theta_1, \ldots, \theta_n$ be the eigenvalues of $S(G)$. Then the following are equivalent:*

(i) $|\det S(G)| \geqslant n - 1$;

(ii) *for any* $0 < \alpha < 2$,

$$|\theta_1|^\alpha + \cdots + |\theta_n|^\alpha \geqslant (n-1)^\alpha + (n-1). \tag{1}$$

The implication '(ii)⇒(i)' is straightforward in view of the fact that

$$\lim_{\alpha \to 0^+} \left(\frac{|\theta_1|^\alpha + \cdots + |\theta_n|^\alpha}{n} \right)^{\frac{1}{\alpha}} = |\theta_1 \cdots \theta_n|^{\frac{1}{n}},$$

which can be verified by taking the natural log and then applying L'Hôpital's rule. We prove the implication '(i)⇒(ii)' in Section 3. The proof is based on KKT method in nonlinear programming. We briefly explain this method in Section 2.

For more results of the same flavor as (1) on Laplacian and signless Laplacian eigenvalues of graphs see [1, 2].

Remark 2. A referee asked whether in Theorem 1, equality in (i) implies equality in (ii). In fact, this is not the case in general. For instance, consider the graph with Seidel matrix

$$S = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & -1 & -1 & -1 \\ 1 & -1 & 0 & -1 & -1 & 1 \\ 1 & -1 & -1 & 0 & 1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 \end{pmatrix}.$$

The eigenvalues of S are $-3.49, -2.23, -.10, 1, 2.23, 2.60$, for which the equality does not hold in (ii) with $\alpha = 1$.

2 Karush–Kuhn–Tucker (KKT) conditions

In nonlinear programming, the Karush–Kuhn–Tucker (KKT) conditions are necessary for a local solution to a minimization problem provided that some regularity conditions are satisfied. Allowing inequality constraints, the KKT approach to nonlinear programming generalizes the method of Lagrange multipliers, which allows only equality constraints. For details see [11].

Consider the following optimization problem:

Minimize $f(\mathbf{x})$
subject to:
$g_j(\mathbf{x}) = 0$, for $j \in J$,
$h_i(\mathbf{x}) \leqslant 0$, for $i \in I$,

where I and J are finite sets of indices. Suppose that the objective function $f : \mathbb{R}^n \to \mathbb{R}$ and the constraint functions $g_j : \mathbb{R}^n \to \mathbb{R}$ and $h_i : \mathbb{R}^n \to \mathbb{R}$ are continuously differentiable at a point $\mathbf{x}^*$. If $\mathbf{x}^*$ is a local minimum that satisfies some regularity conditions, then there exist constants μ_i and λ_j, called KKT multipliers, such that

$$\begin{aligned} \nabla f(\mathbf{x}^*) + \sum_{j \in J} \mu_j \nabla g_j(\mathbf{x}^*) + \sum_{i \in I} \lambda_i \nabla h_i(\mathbf{x}^*) &= \mathbf{0} \\ g_j(\mathbf{x}^*) = 0, &\quad \text{for all } j \in J, \\ h_i(\mathbf{x}^*) \leqslant 0, &\quad \text{for all } i \in I, \\ \lambda_i \geqslant 0, &\quad \text{for all } i \in I, \\ \lambda_i h_i(\mathbf{x}^*) = 0, &\quad \text{for all } i \in I. \end{aligned}$$

In order for a minimum point to satisfy the above KKT conditions, it should satisfy some regularity conditions (or constraint qualifications). The one which suits our problem is the Mangasarian–Fromovitz constraint qualification (MFCQ). Let $I(\mathbf{x}^*)$ be the set of indices of active inequality constraints at $\mathbf{x}^*$, i.e. $I(\mathbf{x}^*) = \{i \in I \mid h_i(\mathbf{x}^*) = 0\}$. We say that MFCQ holds at a feasible point $\mathbf{x}^*$ if the set of gradient vectors $\{\nabla g_j(\mathbf{x}^*) \mid j \in J\}$ is linearly independent and that there exists $\mathbf{w} \in \mathbb{R}^n$ such that

$$\begin{aligned} \nabla g_j(\mathbf{x}^*)\mathbf{w}^\top = 0, &\quad \text{for all } j \in J, \\ \nabla h_i(\mathbf{x}^*)\mathbf{w}^\top < 0, &\quad \text{for all } i \in I(\mathbf{x}^*). \end{aligned}$$

Theorem 3. ([8], see also [11, Section 12.6]) *If a local minimum $\mathbf{x}^*$ of the function $f(\mathbf{x})$ subject to the constraints $g_j(\mathbf{x}) = 0$, for $j \in J$, and $h_i(\mathbf{x}) = 0$, for $i \in I$, satisfies MFCQ, then it satisfies the KKT conditions.*

3 Proof of Theorem 1

In this section we prove the non-trivial part of Theorem 1, that is the implication '(i)⇒(ii)'. We formulate this as an optimization problem. To this end, we need to come up with appropriate constraints. The main constraint is made by the assumption $|\det S(G)| \geqslant n-1$. The other ones are obtained by the following straightforward lemma.

Lemma 4. *For any graph G with n vertices, we have*

(i) $\theta_1(G)^2 + \cdots + \theta_n(G)^2 = (n-1)^2 + n - 1$;

(ii) $\theta_1(G)^4 + \cdots + \theta_n(G)^4 \leqslant \theta_1(K_n)^4 + \cdots + \theta_n(K_n)^4 = (n-1)^4 + n - 1$;

(iii) $\max\limits_{1\leqslant i\leqslant n} \theta_i(G)^2 \leqslant \max\limits_{1\leqslant i\leqslant n} \theta_i(K_n)^2 = (n-1)^2$.

Now, we can describe our problem as the minimization of the function

$$f(\mathbf{x}) := x_1^p + \cdots + x_n^p, \quad \mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n,$$

with fixed $0 < p < 1$, subject to the constraints:

$$g(\mathbf{x}) := x_1 + \cdots + x_n - n(n-1) = 0, \tag{2}$$

$$h(\mathbf{x}) := x_1^2 + \cdots + x_n^2 - (n-1)^4 - (n-1) \leqslant 0, \tag{3}$$

$$d(\mathbf{x}) := (n-1)^2 - \textstyle\prod_{i=1}^n x_i \leqslant 0, \tag{4}$$

$$k_i(\mathbf{x}) := x_i - (n-1)^2 \leqslant 0, \quad \text{for } i = 1, \ldots, n, \tag{5}$$

$$l_i(\mathbf{x}) := \xi - x_i \leqslant 0, \quad \text{for } i = 1, \ldots, n, \tag{6}$$

where $\xi > 0$ is fixed so that if for some i, $x_i = \xi$, then $\prod_{i=1}^n x_i < (n-1)^2$.

Theorem 1 now follows if we prove that the minimum of $f(\mathbf{x})$ subject to (2)–(6) is $(n-1)^{2p} + n - 1$.

Lemma 5. *Let* $\mathbf{e}$ *be a local minimum of* $f(\mathbf{x})$ *subject to the constraints (2)–(6). Then* $\mathbf{e}$ *satisfies MFCQ.*

Proof. Let $\mathbf{e} = (e_1, \ldots, e_n)$. With no loss of generality assume that $e_1 \geqslant \cdots \geqslant e_n$. If $e_1 = e_n$, then, in view of (2), all e_i are equal to $n-1$. In this case, in none of the inequality constraints (3)–(6) equality occurs for $\mathbf{e}$ and so we are done. If $e_1 > e_n$, then MFCQ is fulfilled by setting $\mathbf{w} = (-1, 0, \ldots, 0, 1)$. $\square$

Lemma 6. ([3]) *Suppose $\alpha, \beta, \nu, \omega, a, b, c, d$ are positive numbers and that*

$$\alpha + \beta = \nu + \omega,$$
$$\alpha a + \beta b = \nu c + \omega d,$$
$$\max\{a, b\} \leqslant \max\{c, d\},$$
$$a^\alpha b^\beta \geqslant c^\nu d^\omega.$$

Then the inequality

$$\alpha a^p + \beta b^p \geqslant \nu c^p + \omega d^p$$

holds for $0 \leqslant p \leqslant 1$.

Theorem 7. *Let $\mathbf{e} \in \mathbb{R}^n$ satisfy the constraints (2)–(6). Then $f(\mathbf{e}) \geqslant (n-1)^{2p} + n - 1$.*

Proof. It suffices to prove the assertion for local minima. So assume that $\mathbf{e} = (e_1, \ldots, e_n)$ is a local minimum of $f(\mathbf{x})$ subject to the constraints (2)–(6). Suppose that $e_1 \geqslant \cdots \geqslant e_n$. By Lemma 5, $\mathbf{e}$ satisfies KKT conditions, namely

$$\nabla f(\mathbf{e}) + \mu \nabla g(\mathbf{e}) + \lambda \nabla h(\mathbf{e}) + \delta \nabla d(\mathbf{e}) + \sum_{i=1}^{n} (\rho_i \nabla k_i(\mathbf{e}) + \gamma_i \nabla l_i(\mathbf{e})) = \mathbf{0}, \tag{7}$$

$$e_1 + \cdots + e_n - n(n-1) = 0, \tag{8}$$
$$\lambda \geqslant 0, \quad \lambda h(\mathbf{e}) = 0, \tag{9}$$
$$\delta \geqslant 0, \quad \delta d(\mathbf{e}) = 0,$$
$$\rho_i \geqslant 0, \quad \rho_i k_i(\mathbf{e}) = 0, \quad \text{for } i = 1, \ldots, n, \tag{10}$$
$$\gamma_i \geqslant 0, \quad \gamma_i l_i(\mathbf{e}) = 0, \quad \text{for } i = 1, \ldots, n. \tag{11}$$

By the choice of ξ we have $l_i(\mathbf{e}) < 0$ for $i = 1, \ldots, n$ and hence by (11), $\gamma_1 = \cdots = \gamma_n = 0$. If we let $D = \prod_{i=1}^{n} e_i$, then (7) can be written as

$$pe_i^{p-1} + \mu + 2\lambda e_i - \frac{\delta D}{e_i} + \rho_i = 0, \quad \text{for } i = 1, \ldots, n.$$

We consider the following two cases.

Case 1. $e_1 = (n-1)^2$. Then by (8) and since $\mathbf{e}$ satisfies (4), we have

$$1 = \frac{e_2 + \cdots + e_n}{n-1} \geqslant (e_2 \cdots e_n)^{\frac{1}{n-1}} \geqslant 1.$$

It turns out that $e_2 = \cdots = e_n = 1$ and we are done.

Case 2. $e_1 < (n-1)^2$. So, by (10), $\rho_1 = \cdots = \rho_n = 0$. It turns out that $e_1, \ldots, e_n$ must satisfy the following equation:

$$px^p = \delta D - \mu x - 2\lambda x^2. \tag{12}$$

The curves of $y = px^p$ and $y = \delta D - \mu x - 2\lambda x^2$ intersect in at most two points in $x > 0$ and so (12) has at most two positive roots. If it has one positive root, then by (8), $e_1 = \cdots = e_n = n-1$. Hence $f(\mathbf{e}) = n(n-1)^p$ which is greater than $(n-1)^{2p} + n - 1$ for $n \geqslant 3$. Next assume that (12) has two positive roots, say a and b. These two together with $c = (n-1)^2$ and $d = 1$ satisfy the conditions of Lemma 6. This implies that $f(\mathbf{e}) \geqslant (n-1)^{2p} + n - 1$, completing the proof. □

4 On Seidel matrices with small determinant

We proved that Haemers' conjecture holds for graphs G of order n satisfying $|\det S(G)| \geqslant n-1$. In order to have an intuition on what fraction of graphs does not satisfy this condition, we performed a computation on Seidel matrices up to order $n = 12$. Based on the computation results, we conjecture that this fraction goes to 0 as $n \to \infty$. In connection with this conjecture, we note that almost all graphs of order n have a Seidel energy of $\Theta(n^{3/2})$. As an explicit family of graphs with $|\det S(G)| < n-1$, we prove that self-complementary graphs G of order $n \equiv 1 \pmod 4$ have $\det S(G) = 0$.

We used the databases of non-equivalent Seidel matrices of small orders for our computation. Recall that the *switching class* of a Seidel matrix S is the set of all Seidel matrices $PDSDP^\top$ where P is a permutation matrix and D is a ± 1 diagonal matrix. Two Seidel matrices, S_1 and S_2, are called *switching equivalent*, if $S_2 = PDS_1DP^\top$ holds for some P and D. For $n \leqslant 10$, we made use of the database of Spence [13], for $n = 11$ we used

n	1	2	3	4	5	6	7	8	9	10	11	12
Total	1	1	2	3	7	16	54	243	2038	33120	$1,182,004$	$87,723,296$
# with $\lvert\det\rvert < n-1$	0	0	0	0	1	0	4	6	74	294	3918	89546

Table 1: Numbers of non-equivalent Seidel matrices and those with $|\det| < n-1$ of orders $n \leqslant 12$

Mckay's database of Euler graphs on 11 vertices [9] (note that for odd n, each Seidel switching class contains a unique Euler graph [12], the property which fails for even n [7]), and for $n = 12$ we used the classification given in [5], the database of which is available in [14]. The computation results are summarized in Table 1.

Based on this empirical result, we put forward the following conjecture.

Conjecture. The fraction of graphs G on n vertices with $|\det S(G)| < n-1$ goes to zero as n tends to infinity.

Note that the conjecture implies that Haermers' conjecture is true for almost all graphs. However, as it is shown below, this can be proved independently based on known results. Recall that, the *energy* of a Hermitian matrix M, denoted by $\mathcal{E}(M)$, is sum of the absolute values of eigenvalues of M.

Theorem 8. *For almost all graphs G of order n, $\mathcal{S}(G) = \left(\frac{8}{3\pi} + o(1)\right) n^{3/2}$.*

Proof. For any $n \times n$ complex matrices A, B, by the singular-value inequality of K. Fan [4], we have

$$\sum_{i=1}^{n} s_i(A+B) \leqslant \sum_{i=1}^{n} s_i(A) + \sum_{i=1}^{n} s_i(B),$$

where the singular values of A is denoted by $s_1(A), \ldots, s_n(A)$, etc. Since the singular values of a Hermitian matrix coincides with the absolute values of its eigenvalues, it follows that for Hermitian matrices A, B,

$$\mathcal{E}(A+B) \leqslant \mathcal{E}(A) + \mathcal{E}(B).$$

As $2A(G) = J_n - I_n - S(G)$, we see that

$$2\mathcal{E}(A(G)) \leqslant \mathcal{E}(J_n - I_n) + \mathcal{E}(S(G)) = 2(n-1) + \mathcal{S}(G). \tag{13}$$

Similarly we have

$$\mathcal{S}(G) \leqslant 2(n-1) + 2\mathcal{E}(A(G)). \tag{14}$$

On the other hand, as noted in [10], Wigner's semicircle law [15] implies that for almost all graphs G of order n, $\mathcal{E}(A(G)) = \left(\frac{4}{3\pi} + o(1)\right) n^{3/2}$. This together with (13) and (14) complete the proof. □

We remark that if n is odd and G is a $(n-1)/2$-regular graph then $\det S(G) = 0$ as clearly the all 1's vector is a null vector for $S(G)$. As the final result of the paper, we give another explicit family of graphs G with $|\det S(G)| < n - 1$. Recall that a *self-complementary* graph is a graph isomorphic to its complement. Such graphs can only have orders congruent to 0 or 1 modulo 4.

Theorem 9. *Self-complementary graphs G of order congruent to* 1 *modulo* 4 *have* $\det S(G) = 0$.

Proof. Let G be a self-complementary graph with vertex set $V := \{1, \ldots, n\}$ where $n \equiv 1 \pmod 4$. Also, let $A, \overline{A}$ be the adjacency matrices of $G, \overline{G}$, respectively, and $S := S(G)$. As G is self-complementary, there exists a permutation ρ on V such that $A_{i,j} = 1$ if and only if $\overline{A}_{\rho i, \rho j} = 1$. To prove the assertion, it suffices to show that in the expansion

$$\det S = \sum_{\sigma \in \mathrm{Sym}(V)} \mathrm{sgn}(\sigma) \prod_{i=1}^{n} S_{i,\sigma i}, \tag{15}$$

for any σ, the terms corresponding to σ and $\rho^{-1}\sigma\rho$ have opposite signs.

Let σ be a permutation with no fixed elements, hence $S_{i,\sigma i} = \pm 1$ for $i \in V$. Note that

$$\{(i, \sigma i) \mid i \in V\} = \{(\rho j, \sigma \rho j) \mid j \in V\}.$$

Suppose that $\{V_1, V_2\}$ and $\{V_1', V_2'\}$ are two partitions of V so that $S_{i,\sigma i} = -1$ for $i \in V_1$ and $S_{i,\sigma i} = 1$ for $i \in V_2$, and $\rho(V_1') = V_1$, $\rho(V_2') = V_2$. For $i \in V_1$ we have $S_{i,\sigma i} = -1$, so

$S_{\rho j,\sigma\rho j} = -1$ for $j \in V_1'$. That means, for $j \in V_1'$, $A_{\rho j,\sigma\rho j} = 1$, and hence $\overline{A}_{\rho^{-1}\rho j,\rho^{-1}\sigma\rho j} = 1$ which implies that $S_{j,\rho^{-1}\sigma\rho j} = 1$. Similarly, for $j \in V_2'$ we have $S_{j,\rho^{-1}\sigma\rho j} = -1$. As n is odd, one of $|V_1| = |V_1'|$ or $|V_2| = |V_2'|$ is odd and the other one is even. It follows that $\prod_{i=1}^n S_{i,\sigma i} = -\prod_{i=1}^n S_{i,\rho^{-1}\sigma\rho i}$. As $\mathrm{sgn}(\sigma) = \mathrm{sgn}(\rho^{-1}\sigma\rho)$, the two terms of (15) corresponding to σ and $\rho^{-1}\sigma\rho$ are of opposite signs. This completes the proof. □

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