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CONSTRUCTIONS OF TRACE ZERO SYMMETRIC STOCHASTIC MATRICES FOR THE INVERSE EIGENVALUE PROBLEM*

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Abstract. In the special case of where the spectrum $\sigma = \{\lambda_1, \lambda_2, \lambda_3, 0, 0, \ldots, 0\}$ has at most three nonzero eigenvalues $\lambda_1, \lambda_2, \lambda_3$ with $\lambda_1 \geq 0 \geq \lambda_2 \geq \lambda_3$, and $\lambda_1 + \lambda_2 + \lambda_3 = 0$, the inverse eigenvalue problem for symmetric stochastic $n \times n$ matrices is solved. Constructions are provided for the appropriate matrices where they are readily available. It is shown that when n is odd it is not possible to realize the spectrum σ with an $n \times n$ symmetric stochastic matrix when $\lambda_3 \neq 0$ and $\frac{3}{2n-3} > \frac{\lambda_2}{\lambda_3} \geq 0$, and it is shown that this bound is best possible.

Key words. Inverse eigenvalue problem, Symmetric stochastic matrix, Symmetric nonnegative matrix, Distance matrix.

AMS subject classifications. 15A18, 15A48, 15A51, 15A57

1. Introduction. Let $e_1, \ldots, e_n$ denote the standard basis in $\mathbb{R}^n$, so e_i denotes the vector with a 1 in the ith position and zeroes elsewhere. We will denote by e the vector of all ones, i.e. $e = [1, 1, \ldots, 1]^T \in \mathbb{R}^n$. A matrix $A \in \mathbb{R}^{n\times n}$ is said to be stochastic when all of its entries are nonnegative and all its row sums are equal to 1, i.e. A has right eigenvector e corresponding to the eigenvalue 1. We will be concerned with symmetric stochastic matrices, so that these matrices are in fact doubly stochastic. Also, the eigenvalues will necessarily be real. If $A \in \mathbb{R}^{n\times n}$ is nonnegative, has eigenvalue $\lambda_1 > 0$ corresponding to the right eigenvector e then $\frac{1}{\lambda_1}A$ is stochastic, and for convenience we will state our results in the form, for example, of a matrix A having eigenvector e corresponding to $1 + \epsilon$, where the spectrum $\sigma = \{1 + \epsilon, -1, -\epsilon, 0, 0, \ldots, 0\}$, with $0 \leq \epsilon \leq 1$. We will say that $\sigma = \{\lambda_1, \ldots, \lambda_n\} \subset \mathbb{R}$ is realized as the spectrum of a matrix A in the event that the $n \times n$ matrix A has eigenvalues $\lambda_1, \ldots, \lambda_n$.

The nonnegative inverse eigenvalue problem is to find necessary and sufficient conditions that the elements of the set $\sigma = \{\lambda_1, \ldots, \lambda_n\} \subset \mathbb{C}$ are the eigenvalues of a matrix with nonnegative entries. This problem is currently unsolved except in special cases [1], [7], [8], [9], [10]. The restriction of this problem to symmetric nonnegative matrices for which the eigenvalues $\lambda_1, \ldots, \lambda_n$ satisfy $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$ is solved in [3], where it is shown that the only necessary and sufficient condition is that $\sum_{i=1}^n \lambda_i \geq 0$. Distance matrices are necessarily symmetric, nonnegative, have trace zero, and must have $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$, although these are not sufficient conditions to be a distance matrix. We conjectured in [6], after solving numerous special cases including $n = 2, 3, 4, 5, 6$, that the only necessary and sufficient conditions for the existence of a distance matrix with a given σ is that $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\sum_{i=1}^n \lambda_i = 0$. Distance matrices with eigenvector e were previously studied in [5],

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although not in the context of these matrices eigenvalues. Bounds on the eigenvalues of symmetric stochastic matrices are given in [2] and [4], although they do not provide a restriction on the eigenvalues for the matrices under consideration here.

In Section 2 we provide an explicit construction of an $n \times n$ symmetric stochastic matrix which realizes the spectrum $\{2, -1, -1, 0, 0, \ldots, 0\}$, followed by showing that it is not possible to realize the spectrum $\{1, -1, 0, 0, \ldots, 0\}$ with a symmetric stochastic matrix when n is odd, although it is possible to realize this spectrum when n is even. In Section 3 we provide explicit constructions of symmetric stochastic matrices to realize $\{1 + \epsilon, -1, -\epsilon, 0, 0, \ldots, 0\}$, for $1 \geq \epsilon \geq 0$, when n is even. We then show that it is not possible to realize this spectrum with a symmetric stochastic matrix when $\frac{3}{2n-3} > \epsilon \geq 0$, and n is odd. Although we can realize this spectrum with a symmetric stochastic matrix when $1 \geq \epsilon \geq \frac{3}{2n-3}$, and n is odd. In the latter case we do not provide an explicit construction, instead making use of the Intermediate Value Theorem in several variables.

2. Freedom and restrictions on spectra. Lemma 2.1 will be used to establish that the matrix under consideration is nonnegative.

LEMMA 2.1. *Let $A = (a_{ij}) \in \mathbb{R}^{n \times n}$ be a symmetric matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ which satisfy $\lambda_1 \geq 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Suppose that A has eigenvector e corresponding to λ_1, and that A has all diagonal entries equal to zero. Then A is a nonnegative matrix.*

Proof. Write $A = \lambda_1 \frac{ee^T}{n} + \lambda_2 u_2 u_2^T + \cdots + \lambda_n u_n u_n^T$, where $u_2, \ldots, u_n$ are unit eigenvectors corresponding to $\lambda_2, \ldots, \lambda_n$, respectively. Then $-2a_{ij} = (e_i - e_j)^T A (e_i - e_j) = \lambda_2((e_i - e_j)^T u_2)^2 + \cdots + \lambda_n((e_i - e_j)^T u_n)^2 \leq 0$, for all i, j, $1 \leq i, j \leq n$. □

Our next two theorems give some foretaste of what is and isn't possible with the inverse eigenvalue problem for symmetric nonnegative matrices. Note first that a 3×3 symmetric nonnegative matrix with eigenvector e and of trace zero must be a nonnegative scalar multiple of $A = ee^T - I$, which has spectrum $\sigma = \{2, -1, -1\}$.

THEOREM 2.2. *Let $\sigma = \{2, -1, -1, 0, 0, \ldots, 0\}$. Then σ can be realized as the spectrum of a symmetric nonnegative matrix $A \in \mathbb{R}^{n \times n}$ with eigenvector e corresponding to 2, for $n \geq 3$.*

Proof. Let $u = [u_1, \ldots, u_n]^T, v = [v_1, \ldots, v_n]^T \in \mathbb{R}^n$ be given by $u_j = \sqrt{\frac{2}{n}} \cos\, \theta_j$, $v_j = \sqrt{\frac{2}{n}} \sin\, \theta_j$, where $\theta_j = \frac{2\pi}{n} j$, for $1 \leq j \leq n$. Then $A = 2\frac{ee^T}{n} - uu^T - vv^T$ is symmetric and has zero diagonal entries by construction. Since the roots of $x^n - 1$ are $e^{\frac{2\pi i}{n} j}$, $1 \leq j \leq n$, then (coefficient of x^{n-1}) $= 0 = \sum_{j=1}^n -e^{\frac{2\pi i}{n} j}$ and (coefficient of x^{n-2}) $= 0 = \sum_{j,k=1, j \neq k}^n e^{\frac{2\pi i}{n} j} e^{\frac{2\pi i}{n} k} = (\sum_{j=1}^n e^{\frac{2\pi i}{n} j})^2 - \sum_{j=1}^n e^{\frac{2\pi i}{n} 2j}$. It follows that $\sum_{j=1}^n \cos\, \theta_j = \sum_{j=1}^n \sin\, \theta_j = \sum_{j=1}^n \sin\, 2\theta_j = 0$, which tells us that $u^T e = v^T e = u^T v = 0$, respectively. It also follows that $\sum_{j=1}^n \cos\, 2\theta_j = 0$, so that $\sum_{j=1}^n \cos^2\, \theta_j - \sum_{j=1}^n \sin^2\, \theta_j = 0$. We also know that $\sum_{j=1}^n \cos^2\, \theta_j + \sum_{j=1}^n \sin^2\, \theta_j = n$, so we can conclude that $\sum_{j=1}^n \cos^2\, \theta_j = \sum_{j=1}^n \sin^2\, \theta_j = \frac{n}{2}$. This tells us that u and v are unit vectors. Thus A has spectrum σ and is nonnegative from Lemma 2.1. □

THEOREM 2.3. *Let $\lambda_1 > 0$ and $\sigma = \{\lambda_1, -\lambda_1, 0, \ldots, 0\}$. Then σ cannot be realized as the spectrum of an $n \times n$ symmetric nonnegative matrix with eigenvector*

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e corresponding to λ_1, when n is odd.

Proof. Suppose A is a matrix of the given form that realizes σ. Write $A = \lambda_1 \frac{ee^T}{n} - \lambda_1 uu^T$, where $u = [u_1, \ldots, u_n]^T \in \mathbb{R}^n$, $||u|| = 1$ and $u^T e = 0$. A has trace zero and is nonnegative by hypothesis so all diagonal entries are zero, and thus $0 = \frac{\lambda_1}{n} - \lambda_1 u_i^2$, for $1 \le i \le n$. But then $u_i = \frac{\pm 1}{\sqrt{n}}$ and $0 = \sum_{i=1}^n u_i = \sum_{i=1}^n \frac{\pm 1}{\sqrt{n}}$, which is not possible when n is odd. □

REMARK 2.4. The same σ of Theorem 2.3 can be realized by an $n \times n$ symmetric nonnegative matrix with eigenvector e corresponding to λ_1 when n is even, by taking in the proof the unit vector $u = \frac{1}{\sqrt{n}}[1, 1, \ldots, 1, -1, -1, \ldots, -1]^T \in \mathbb{R}^n$.

3. At most three nonzero eigenvalues. The idea in Remark 2.4 can be extended to the case where n is a multiple of 4 for the case of at most three nonzero eigenvalues.

THEOREM 3.1. *Let $\sigma = \{1 + \epsilon, -1, -\epsilon, 0, 0, \ldots, 0\}$, where $1 \ge \epsilon \ge 0$. Then σ can be realized by a symmetric nonnegative matrix $A \in \mathbb{R}^{n \times n}$ with eigenvector e corresponding to $1 + \epsilon$, when $n = 4m$ for some m.*

Proof. Let $u, v \in \mathbb{R}^n$ be given by

$$u = \frac{1}{\sqrt{n}}[1, 1, \ldots, 1, \ \ 1, \ \ 1, \ldots, \ \ 1, -1, -1, \ldots, -1, -1, -1, \ldots, -1]^T,$$
$$v = \frac{1}{\sqrt{n}}[1, 1, \ldots, 1, -1, -1, \ldots, -1, \ \ 1, \ \ 1, \ldots, \ \ 1, -1, -1, \ldots, -1]^T.$$

Then $\frac{e}{\sqrt{n}}$, u and v are orthonormal. Let $A = \frac{(1+\epsilon)}{n} ee^T - uu^T - \epsilon vv^T$, and note that all the diagonal entries of A are zero. □

However, the way we deal with the remaining cases for n even is somewhat more complicated.

THEOREM 3.2. *Let $\sigma = \{1 + \epsilon, -1, -\epsilon, 0, 0, \ldots, 0\}$, where $1 \ge \epsilon \ge 0$. Then σ can be realized by a symmetric nonnegative matrix $A \in \mathbb{R}^{n \times n}$ with eigenvector e corresponding to $1 + \epsilon$, when $n = 4m + 2$ for some m.*

Proof. Let $u = [u_1, \ldots, u_n]^T$, $v = [v_1, \ldots, v_n]^T \in \mathbb{R}^n$, and $A = (1 + \epsilon)\frac{ee^T}{n} - uu^T - \epsilon vv^T$. We will require that $0 = \frac{1+\epsilon}{n} - u_i^2 - \epsilon v_i^2$, for $1 \le i \le n$, so that A has all zero diagonal entries. Let $u_i = \sqrt{\frac{1+\epsilon}{n}} \cos \theta_i$ and $v_i = \sqrt{\frac{1+\epsilon}{n\epsilon}} \sin \theta_i$, where the θ_i's are chosen below. Our θ_i's must satisfy $\sum_{i=1}^n \cos \theta_i = \sum_{i=1}^n \sin \theta_i = \sum_{i=1}^n \cos \theta_i \sin \theta_i = 0$. So that u and v are unit vectors we must have $\sum_{i=1}^n \cos^2 \theta_i = \frac{n}{1+\epsilon}$ and $\sum_{i=1}^n \sin^2 \theta_i = \frac{n\epsilon}{1+\epsilon}$, which will be achieved if $\sum_{i=1}^n \cos^2 \theta_i - \sum_{i=1}^n \sin^2 \theta_i = \frac{n(1-\epsilon)}{1+\epsilon}$, and $\sum_{i=1}^n \cos^2 \theta_i + \sum_{i=1}^n \sin^2 \theta_i = n$. So for any given $\epsilon \in [0, 1]$ we also require for our choice of θ_i's that $\sum_{i=1}^n \cos 2\theta_i = \frac{n(1-\epsilon)}{1+\epsilon}$.

Let $0 \le \delta < \frac{2\pi}{n}$, and choose the angles θ_i, $1 \le i \le n$, around the origin in the plane.

Let θ_i for $1 \le i \le m$ be, respectively, the 1st quadrant angles

$$\frac{2\pi}{n} - \delta, \ 2(\frac{2\pi}{n} - \delta), \ldots, (m-1)(\frac{2\pi}{n} - \delta), m(\frac{2\pi}{n} - \delta).$$

Let θ_i for $m + 1 \le i \le 2m$ be, respectively, the 2nd quadrant angles

$$(m+1)\frac{2\pi}{n} + m\delta, \ (m+2)\frac{2\pi}{n} + (m-1)\delta, \ldots, (2m-1)\frac{2\pi}{n} + 2\delta, 2m\frac{2\pi}{n} + \delta.$$

Let $\theta_{2m+1} = \pi$.

Let θ_i for $2m + 2 \le i \le 3m + 1$ be, respectively, the 3rd quadrant angles

$$-2m\frac{2\pi}{n} - \delta, \ -(2m-1)\frac{2\pi}{n} - 2\delta, \ldots, -(m+2)\frac{2\pi}{n} - (m-1)\delta, -(m+1)\frac{2\pi}{n} - m\delta.$$

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Let θ_i for $3m+2 \le i \le 4m+1$ be, respectively, the 4th quadrant angles
$-m(\frac{2\pi}{n}-\delta),\ -(m-1)(\frac{2\pi}{n}-\delta), \ldots, -2(\frac{2\pi}{n}-\delta), -(\frac{2\pi}{n}-\delta)$.

Let $\theta_{4m+2}=0$.

For each θ_i there is a $\theta_i+\pi$ in the above list, by pairing off 1st quadrant angles with appropriate 3rd quadrant angles, and pairing 2nd quadrant angles with appropriate 4th quadrant angles. Therefore since $\cos\,(\theta_i+\pi) = -\cos\,\theta_i$ we conclude that $\sum_{i=1}^n \cos\,\theta_i = 0$.

For each $\theta_i \ne 0$ and $\theta_i \ne \pi$ in the above list we can pair off any θ_i with a corresponding $-\theta_i$ and conclude that $\sum_{i=1}^n \sin\,\theta_i = 0$.

Similarly, $\sum_{i=1}^n \sin\,2\theta_i = 0$.

Pairing off each θ_i with a $\theta_i+\pi$ in the same way as before, and since $\cos\,2\theta_i = \cos\,(2\theta_i+2\pi)$, we must have

$$\sum_{i=1}^n \cos\,2\theta_i = 2 + \sum_{\text{1st,2nd,3rd,4th quadrant}} \cos\,2\theta_i = 2 + 2\sum_{\text{1st,4th quadrant}} \cos\,2\theta_i.$$

Because we can pair off each θ_i in the 1st quadrant with each $-\theta_i$ in the 4th quadrant $\sum_{i=1}^n \cos\,2\theta_i = 2 + 4\sum_{\text{1st quadrant}} \cos\,2\theta_i$. Next using the trigonometric formula

$$\sum_{j=0}^n \cos\,j\alpha = \frac{\sin\,(\frac{n+1}{2}\alpha)\,\cos\,(\frac{n}{2}\alpha)}{\sin\,\frac{\alpha}{2}}$$

(found in [11], for example), where $\alpha = 2(\frac{2\pi}{n}-\delta)$ and some simplification we obtain that $\sum_{i=1}^n \cos\,2\theta_i = 2\,\frac{\sin\,((2m+1)\delta)}{\sin\,(\frac{\pi}{2m+1}-\delta)}$. Let $f(\delta) = 2\,\frac{\sin\,((2m+1)\delta)}{\sin\,(\frac{\pi}{2m+1}-\delta)}$, then $f(0)=0$ and $\lim_{\delta\to\frac{2\pi}{n}} f(\delta) = n$, and notice that f is continuous on the interval $[0,\frac{2\pi}{n})$. Also, since $0 \le \epsilon \le 1$ we have that $0 \le \frac{n(1-\epsilon)}{1+\epsilon} \le n$, but then by the Intermediate Value Theorem for each $\epsilon \in (0,1]$ there is a $\delta \in [0,\frac{2\pi}{n})$ such that $f(\delta) = \frac{n(1-\epsilon)}{1+\epsilon}$. The case $\epsilon = 0$ and $\delta = \frac{2\pi}{n}$ is covered by the remark after Theorem 2.3. □

In order to deal with the case where n is odd we will improve on Theorem 2.3.

THEOREM 3.3. *Let $\sigma = \{1+\epsilon, -1, -\epsilon, 0, 0, \ldots, 0\}$, where $\frac{3}{2n-3} > \epsilon \ge 0$, and $n \ge 3$. Then σ cannot be realized by a symmetric nonnegative matrix $A \in \mathbb{R}^{n\times n}$ with eigenvector e corresponding to $1+\epsilon$, when $n = 2m+1$ for some m.*

Proof. σ is realizable when $\epsilon = 1$ from Theorem 2.2. We wish to determine the minimum value of ϵ for which it is possible to construct a matrix of the desired form. Using the same notation as in the proof of Theorem 3.2 we wish to determine the minimum value of ϵ as a function of $\theta_1, \ldots, \theta_n$ subject to the three constraints $\sum_{i=1}^n \cos\,\theta_i = \sum_{i=1}^n \sin\,\theta_i = 0$ and $\sum_{i=1}^n \cos\,\theta_i \sin\,\theta_i = 0$ (we know from Theorem 2.3 that $\epsilon > 0$). Observe that finding the minimum ϵ is equivalent to finding the maximum value of the function $\frac{n}{1+\epsilon} = F(\theta_1, \ldots, \theta_n) = \sum_{i=1}^n \cos^2\,\theta_i$ subject to the three constraints. For the moment let us determine the maximum value of F subject to the one constraint $\sum_{i=1}^n \cos\,\theta_i = 0$. Let λ denote the Lagrange multiplier so that $-2\cos\,\theta_i \sin\,\theta_i - \lambda \sin\,\theta_i = 0$, i.e. $\sin\,\theta_i(2\cos\,\theta_i + \lambda) = 0$, for each i, $1 \le i \le n$. Then

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for each i we have $\sin\,\theta_i = 0$ or else $\cos\,\theta_i = -\lambda/2$. We cannot have all θ_i's equal to 0 or π, since then we would not have $\sum_{i=1}^n \cos\,\theta_i = 0$, because n is odd. Suppose now that k of the $\cos\,\theta_i$'s are equal, but not equal to ± 1, then $k\,\cos\,\theta_i = \pm 1 \pm 1 \cdots$. Then in order to maximize F we must have as many ± 1's as possible, thus we must have $k = 2$ with $\cos\,\theta_p = \cos\,\theta_q$ (say) and the remaining θ_i's all either 0 or π. Then $2\,\cos\,\theta_i = 1$ or -1, and there are two possibilities:
Case 1: $\cos\,\theta_p = \cos\,\theta_q = \frac{1}{2}$ with $m-1$ of the remaining $\cos\,\theta_i$'s equal to 1 and the other m of the $\cos\,\theta_i$'s equal to -1.
Case 2: $\cos\,\theta_p = \cos\,\theta_q = -\frac{1}{2}$ with $m-1$ of the remaining $\cos\,\theta_i$'s equal to -1 and the other m of the $\cos\,\theta_i$'s equal to 1.

In either case the maximum value of F is $\frac{1}{2} + 2m - 1 = n - \frac{3}{2}$, in which case $\epsilon = \frac{3}{2n-3}$.

Notice now that this maximum value for F can be just as easily achieved when $\theta_p = -\theta_q$ and that then $\sum_{i=1}^n \sin\,\theta_i = 0$ and $\sum_{i=1}^n \cos\,\theta_i\,\sin\,\theta_i = 0$. So ϵ has in effect been minimized subject to all three constraints. □

COROLLARY 3.4. *Let $\sigma = \{1+\epsilon, -1, -\epsilon, 0, \ldots, 0\}$, where $1 \geq \epsilon \geq \frac{3}{2n-3}$, and $n \geq 3$. Then σ can realized as the spectrum of a symmetric nonnegative matrix $A \in \mathbb{R}^{n\times n}$ with eigenvector e corresponding to $1+\epsilon$, when n is odd.*

Proof. Let $F(\theta_1, \ldots, \theta_n) = \sum_{j=1}^n \cos^2\,\theta_j$. Then

$$F(\frac{2\pi}{n}1, \frac{2\pi}{n}2, \ldots, \frac{2\pi}{n}(n-1), \frac{2\pi}{n}n) = \frac{n}{2},$$

and

$$F(\frac{2\pi}{3}, -\frac{2\pi}{3}, 0, 0, \ldots, 0, \pi, \pi, \ldots, \pi) = n - \frac{3}{2}.$$

Moreover, F is continuous as a function of $\cos\,\theta_1, \ldots, \cos\,\theta_n$, particularly on the following intervals for the $\cos\,\theta_i$'s:

For $n = 4k+3$ let the $\cos\,\theta_i$'s satisfy $\cos\frac{2\pi(k+1)}{n} \leq \cos\,\theta_{k+1} \leq \cos\frac{2\pi}{3}$ and $\cos\frac{2\pi(3k+3)}{n} \leq \cos\,\theta_{3k+3} \leq \cos\frac{2\pi}{3}$. Also, let $\cos\frac{2\pi}{n}j \leq \cos\,\theta_j \leq \cos 0$ for $1 \leq j \leq k$ and $3k+4 \leq j \leq 4k+3$, and let $\cos\,\pi \leq \cos\,\theta_j \leq \cos\frac{2\pi}{n}j$ for $k+2 \leq j \leq 3k+2$ except that $\cos\,\theta_{2k+2} = \cos\,\pi$.

For $n = 4k+1$ let the $\cos\,\theta_i$'s satisfy $\cos\frac{2\pi(k+1)}{n} \leq \cos\,\theta_{k+1} \leq \cos\frac{2\pi}{3}$ and $\cos\frac{2\pi(3k+2)}{n} \leq \cos\,\theta_{3k+2} \leq \cos\frac{2\pi}{3}$. Also, let $\cos\frac{2\pi}{n}j \leq \cos\,\theta_j \leq \cos 0$ for $1 \leq j \leq k$ and $3k+3 \leq j \leq 4k+1$, and let $\cos\,\pi \leq \cos\,\theta_j \leq \cos\frac{2\pi}{n}j$ for $k+2 \leq j \leq 3k+1$ except that $\cos\,\theta_1 = \cos 0$.

For each ϵ such that $1 \geq \epsilon \geq \frac{3}{2n-3}$ we have $\frac{n}{2} \leq \frac{n}{1+\epsilon} \leq n - \frac{3}{2}$, then from the Intermediate Value Theorem for real valued functions of several variables it follows that for each $\epsilon \in [\frac{3}{2n-3}, 1]$ there is a $(\theta_1, \ldots, \theta_n)$ such that $F(\theta_1, \ldots, \theta_n) = \frac{n}{1+\epsilon}$. □

The author does not see a natural extension of the above methods to deal with the case of at most four nonzero eigenvalues.

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