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EXTREMAL EIGENVALUES OF REAL SYMMETRIC MATRICES WITH ENTRIES IN AN INTERVAL*

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Abstract. We determine the exact range of the smallest and largest eigenvalues of real symmetric matrices of a given order whose entries are in a given interval. The maximizing and minimizing matrices are specified. We also consider the maximal spread of such matrices.

Key words. eigenvalue, symmetric matrix, spread

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1. Introduction. Let $S_n[a,b]$ denote the set of $n \times n$ real symmetric matrices whose entries are in the interval $[a, b]$. For an $n \times n$ real symmetric matrix A, we always denote the eigenvalues of A in decreasing order by $\lambda_1(A) \geq \cdots \geq \lambda_n(A)$. We will study the smallest eigenvalue $\lambda_n(A)$ and the largest eigenvalue $\lambda_1(A)$ when A varies in $S_n[a,b]$. Constantine [2] proved that if $A \in S_n[0,b]$, then

$$\lambda_n(A) \geq \begin{cases} -nb/2 & \text{if } n \text{ is even,} \\ -\sqrt{n^2-1}b/2 & \text{if } n \text{ is odd.} \end{cases}$$

So the matrices treated there are nonnegative. The proof techniques of [2] are graph-theoretic. In [7] Roth gave another proof of this result by analysis of eigenvectors.

In this paper we will determine the smallest and largest values of both $\lambda_n(A)$ and $\lambda_1(A)$ when $A \in S_n[a,b]$ for generic $a < b$, thus generalizing Constantine's result.

The spread of an $n \times n$ real symmetric matrix A is defined as $s(A) = \lambda_1(A) - \lambda_n(A)$. This quantity has applications in combinatorial optimization problems [3]. Some lower bounds on the spread of Hermitian matrices are known; see [5] and the references therein. We will determine the maximal value of $s(A)$ for $A \in S_n[-a,a]$.

We always regard real vectors in $\mathbb{R}^n$ as $n \times 1$ matrices. A basic fact (see [1] or [4]) for an $n \times n$ real symmetric matrix A is

$$\lambda_n(A) = \min\{x^T Ax : \|x\| = 1, x \in \mathbb{R}^n\}, \quad \lambda_1(A) = \max\{x^T Ax : \|x\| = 1, x \in \mathbb{R}^n\}.$$

2. Extremal eigenvalues. We first consider the lower bound for the smallest eigenvalue. Denote by $J_{r,s}$ the $r \times s$ matrix with all entries equal to 1, and write J_r for $J_{r,r}$.

THEOREM 1. *Let $A \in S_n[a,b]$ with $n \geq 2$ and $a < b$.*

(i) *If $|a| < b$, then*

$$\lambda_n(A) \geq \begin{cases} n(a-b)/2 & \text{if } n \text{ is even,} \\ \left(na - \sqrt{a^2+(n^2-1)b^2}\right)/2 & \text{if } n \text{ is odd.} \end{cases}$$

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If n is even, equality holds if and only if A is permutation similar to

$$\begin{bmatrix} a & b \\ b & a \end{bmatrix} \otimes J_{\frac{n}{2}}.$$

If n is odd, equality holds if and only if A is permutation similar to

$$\begin{bmatrix} aJ_{\frac{n-1}{2}} & bJ_{\frac{n-1}{2},\frac{n+1}{2}} \\ bJ_{\frac{n+1}{2},\frac{n-1}{2}} & aJ_{\frac{n+1}{2}} \end{bmatrix}.$$

(ii) *If $|a| \geq b$, then $\lambda_n(A) \geq na$. If $|a| > b$, equality holds if and only if $A = aJ_n$. If $|a| = b$, equality holds if and only if A is permutation similar to*

$$\begin{bmatrix} aJ_k & bJ_{k,n-k} \\ bJ_{n-k,k} & aJ_{n-k} \end{bmatrix}$$

for some k with $1 \leq k \leq n$.

Proof. For any fixed $A \in S_n[a,b]$, let $x = (x_1, \ldots, x_n)^T$ be a unit (i.e., $\|x\| = 1$) eigenvector corresponding to $\lambda_n(A)$. By simultaneous permutations of the rows and columns of A if necessary, we may suppose that $x_i \geq 0$ for $i = 1, \ldots, k$ and $x_j < 0$ for $j = k+1, \ldots, n$, $1 \leq k \leq n$. We need not consider the case $k = 0$, as in that case we use $-x$ instead of x. Let $e \in \mathbb{R}^n$ be the vector with all entries equal to 1. Denote by $A \circ B$ the Hadamard product of A and B, i.e., the entrywise product. Then we may write $x^T Ax$ in a more visible form:

$$\lambda_n(A) = x^T Ax = e^T[A \circ (xx^T)]e. \tag{1}$$

Note that the matrix xx^T is divided into four blocks: The entries in $(xx^T)[1, \ldots, k]$ and in $(xx^T)[k+1, \ldots, n]$ are nonnegative, while the entries in $(xx^T)[1, \ldots, k|k+1, \ldots, n]$ and in $(xx^T)[k+1, \ldots, n|1, \ldots, k]$ are nonpositive. Thus from (1) we see clearly that if we define

$$\tilde{A} = J(k; a, b) \equiv \begin{bmatrix} aJ_k & bJ_{k,n-k} \\ bJ_{n-k,k} & aJ_{n-k} \end{bmatrix}, \tag{2}$$

then

$$\lambda_n(\tilde{A}) = \min\{y^T \tilde{A} y : \|y\| = 1, y \in \mathbb{R}^n\} \leq x^T \tilde{A} x \leq x^T Ax = \lambda_n(A).$$

Therefore the smallest value of $\lambda_n(A)$ for $A \in S_n[a,b]$ can be attained at some matrix of the form in (2). Since the rank of $J(k; a, b)$ is at most 2, it has at most two nonzero eigenvalues. By considering the trace and the Frobenius norm we deduce that

$$\lambda_n(J(k; a, b)) = \left(na - \sqrt{(n-2k)^2 a^2 + 4k(n-k)b^2}\right)/2. \tag{3}$$

(i) Since $|a| < b$, if n is even, the right side of (3) attains its minimum at $k = n/2$ and

$$\lambda_n(A) \geq \lambda_n(J(n/2; a, b)) = n(a-b)/2$$

for any $A \in S_n[a,b]$. If n is odd, the right side of (3) attains its minimum at $k = (n-1)/2$ and $k = (n+1)/2$. Hence

$$\lambda_n(A) \geq \lambda_n(J((n-1)/2; a, b)) = \left(na - \sqrt{a^2 + (n^2-1)b^2}\right)/2.$$

Now we prove the equality conditions. First suppose n is even. Let $A = (a_{ij}) \in S_n[a,b]$ such that $\lambda_n(A) = n(a-b)/2$ and let $x = (x_1, \ldots, x_n)^T$ be a corresponding unit eigenvector. Suppose x has exactly t nonzero components with $t < n$. By the above bounds, if t is even, then

$$\lambda_n(A) = x^T Ax \geq t(a-b)/2 > n(a-b)/2,$$

and if t is odd, then

$$\lambda_n(A) = x^T Ax \geq \left(ta - \sqrt{(a^2-b^2)+t^2b^2}\right)/2 > t(a-b)/2 > n(a-b)/2,$$

both contradicting the assumption that $\lambda_n(A) = n(a-b)/2$. Therefore all the components of x are nonzero. Suppose x has k positive components and $n-k$ negative components. From (3) we know that if $k \neq n/2$,

$$\lambda_n(A) \geq \lambda_n(J(k;a,b)) > \lambda_n(J(n/2;a,b)) = n(a-b)/2,$$

a contradiction. Thus we must have $k = n/2$. By simultaneous row and column permutations of A if necessary, we may suppose that $x_i > 0$ for $i = 1, \ldots, n/2$ and $x_j < 0$ for $j = (n/2)+1, \ldots, n$. Then

$$\lambda_n(A) = x^T Ax \geq x^T J(n/2;a,b)x \geq \lambda_n(A)$$

forces $A = J(n/2;a,b)$, since otherwise the first inequality above will be strict, which is impossible. Therefore the original A is permutation similar to $J(n/2;a,b)$.

The equality condition for the case when n is odd can be similarly proved. Just note that

$$t(a-b) > na - \sqrt{a^2+(n^2-1)b^2}$$

for $1 \leq t \leq n-1$, the lower bound $(na - \sqrt{a^2+(n^2-1)b^2})/2$ is strictly decreasing in n, and

$$\begin{bmatrix} aJ_{\frac{n+1}{2}} & bJ_{\frac{n+1}{2},\frac{n-1}{2}} \\ bJ_{\frac{n-1}{2},\frac{n+1}{2}} & aJ_{\frac{n-1}{2}} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} aJ_{\frac{n-1}{2}} & bJ_{\frac{n-1}{2},\frac{n+1}{2}} \\ bJ_{\frac{n+1}{2},\frac{n-1}{2}} & aJ_{\frac{n+1}{2}} \end{bmatrix}$$

are permutation similar.

(ii) $|a| \geq b$ and $a < b$ imply $a < 0$. If $|a| > b$, the minimum of the right side of (3) is attained at $k = n$, and if $|a| = b$, the right side of (3) has equal values for all k with $1 \leq k \leq n$. In any case the minimum is na. This proves $\lambda_n(A) \geq na$. The proof of the equality conditions is similar to that of case (i) and we omit the details. □

Since $A \in S_n[a,b]$ implies $A - aJ_n \in S_n[0, b-a]$, it is natural to ask whether Theorem 1 can be deduced from Constantine's result by using the perturbation inequality: $\lambda_n(G+H) \geq \lambda_n(G) + \lambda_n(H)$ for $n \times n$ real symmetric matrices G, H [1]. In general the answer is no. Let us examine the case $0 < a < b$. If n is odd, the perturbation inequality and Constantine's result give

$$\begin{aligned} \lambda_n(A) &= \lambda_n[(A - aJ_n) + aJ_n] \\ &\geq \lambda_n(A - aJ_n) + \lambda_n(aJ_n) \\ &= \lambda_n(A - aJ_n) \\ &\geq \sqrt{n^2-1}(a-b)/2. \end{aligned}$$

It is easy to verify that this lower bound $\sqrt{n^2-1}(a-b)/2$ is strictly less than the sharp bound $(na - \sqrt{a^2+(n^2-1)b^2})/2$ in Theorem 1. On the other hand, if n is even, the lower bound $n(a-b)/2$ can indeed be deduced from Constantine's result.

For a real $n \times n$ symmetric matrix A, $\lambda_1(A) = -\lambda_n(-A)$. Also $a \le a_{ij} \le b$ is equivalent to $-b \le -a_{ij} \le -a$. Thus the following corollary on upper bounds for the largest eigenvalue follows from Theorem 1.

Corollary 2. *Let $A \in S_n[a,b]$ with $n \ge 2$ and $a < b$.*

(i) *If $a < -|b|$, then*

$$\lambda_1(A) \le \begin{cases} n(b-a)/2 & \text{if } n \text{ is even,} \\ \left(nb + \sqrt{b^2+(n^2-1)a^2}\right)/2 & \text{if } n \text{ is odd.} \end{cases}$$

If n is even, equality holds if and only if A is permutation similar to

$$\begin{bmatrix} b & a \\ a & b \end{bmatrix} \otimes J_{\frac{n}{2}}.$$

If n is odd, equality holds if and only if A is permutation similar to

$$\begin{bmatrix} bJ_{\frac{n-1}{2}} & aJ_{\frac{n-1}{2},\frac{n+1}{2}} \\ aJ_{\frac{n+1}{2},\frac{n-1}{2}} & bJ_{\frac{n+1}{2}} \end{bmatrix}.$$

(ii) *If $a \ge -|b|$, then $\lambda_1(A) \le nb$. If $a > -|b|$, equality holds if and only if $A = bJ_n$. If $a = -|b|$, equality holds if and only if A is permutation similar to*

$$\begin{bmatrix} bJ_k & aJ_{k,n-k} \\ aJ_{n-k,k} & bJ_{n-k} \end{bmatrix}$$

for some k with $1 \le k \le n$.

Now we turn to the study of upper bounds on the smallest eigenvalue and lower bounds on the largest eigenvalue. For real matrices A, B, we write $A \le B$ to mean that $B - A$ is entrywise nonnegative. We need the following two lemmas.

Lemma 3 (see [1] or [4]). *Let H be a real symmetric matrix of order n and G be a principal submatrix of order k of H. Then*

$$\lambda_j(H) \ge \lambda_j(G) \ge \lambda_{j+n-k}(H)$$

for $j = 1, \ldots, k$.

Lemma 4 (see [6, p. 38]). *Let A, B be nonnegative matrices of the same order satisfying $A \le B$. Then $\rho(A) \le \rho(B)$, where $\rho(\cdot)$ is the Perron root (spectral radius). If, in addition, $A \ne B$ and B is irreducible, then $\rho(A) < \rho(B)$.*

Since $\lambda_n(A) = -\lambda_1(-A)$ and $\lambda_1(A) = -\lambda_n(-A)$ for $n \times n$ real symmetric matrices A, for our problem there are essentially two different cases: $0 < a < b$ and $a \le 0 < b$. Denote by J and I the $n \times n$ all-one matrix and the $n \times n$ identity matrix, respectively.

Theorem 5. *Let $A \in S_n[a,b]$ with $n \ge 2$ and $a < b$.*

(i) *Let $0 < a < b$. Then*

$$\lambda_n(A) \le b - a. \tag{4}$$

Equality in (4) holds if and only if $A = aJ + (b-a)I$.

$$\lambda_1(A) \ge na. \tag{5}$$

Equality in (5) holds if and only if $A = aJ$.

(ii) *Let* $a \le 0 < b$. *Then*

$$\lambda_n(A) \le b. \tag{6}$$

Equality in (6) *holds if and only if* $A = bI$.

$$\lambda_1(A) \ge a. \tag{7}$$

Equality in (7) *holds if and only if* $A = aI$.

Proof. (i) Let $A = (a_{ij})$. For $i < j$, by Lemma 3 we have

$$\begin{aligned}\lambda_n(A) \le \lambda_2\left(\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj}\end{bmatrix}\right) &= \frac{a_{ii}+a_{jj}-\sqrt{(a_{ii}-a_{jj})^2+4a_{ij}^2}}{2} \\ &\le \frac{a_{ii}+a_{jj}-2a_{ij}}{2} \le b-a. \end{aligned} \tag{8}$$

Thus $\lambda_n(A) \le b-a$. If $\lambda_n(A) = b-a$, all the inequalities in (8) must be equality. This forces $a_{ii} = a_{jj} = b$ and $a_{ij} = a_{ji} = a$. As this should be true for all $i < j$, $A = aJ + (b-a)I$.

$A \in S_n[a,b]$ implies $A \ge aJ \ge 0$. By Lemma 4 and the Perron–Frobenius theory [6],

$$\lambda_1(A) = \rho(A) \ge \rho(aJ) = \lambda_1(aJ) = na.$$

If $A \in S_n[a,b]$ and $A \ne aJ$, then since A is irreducible (A is in fact entrywise positive), again by Lemma 4, $\lambda_1(A) > \lambda_1(aJ) = na$. Thus $\lambda_1(A) = na$ if and only if $A = aJ$.

(ii)

$$\lambda_n(A) \le \frac{\mathrm{tr}A}{n} \le \frac{nb}{n} = b.$$

If $\lambda_n(A) = b$, then $\mathrm{tr}A = nb$ and consequently $a_{ii} = b$, $i = 1, \dots, n$. For any $i < j$, by Lemma 3 we have

$$b = \lambda_n(A) \le \lambda_2\left(\begin{bmatrix} b & a_{ij} \\ a_{ji} & b\end{bmatrix}\right) = b - |a_{ij}|.$$

Thus $a_{ij} = 0$ for all $i < j$, i.e., $A = bI$.

$$\lambda_1(A) \ge \frac{\mathrm{tr}A}{n} \ge \frac{na}{n} = a.$$

If $\lambda_1(A) = a$, then $\mathrm{tr}A = na$ and hence $a_{ii} = a$, $i = 1, \dots, n$. For any $i < j$, by Lemma 3 we have

$$a = \lambda_1(A) \ge \lambda_1\left(\begin{bmatrix} a & a_{ij} \\ a_{ji} & a\end{bmatrix}\right) = a + |a_{ij}|.$$

So $a_{ij} = 0$ for all $i < j$, i.e., $A = aI$. This completes the proof. $\square$

3. The maximal spread. Denote by $s(A)$ the spread of A. We treat only the case when the interval is symmetric about the origin. Of course we may use the upper bound on λ_1 in Corollary 2 and the lower bound on λ_n in Theorem 1 to give an upper bound on the spread $\lambda_1 - \lambda_n$, but that bound is not sharp. This is because the upper bound on λ_1 and the lower bound on λ_n cannot be simultaneously attained at one common matrix.

A $\{\pm 1\}$-*matrix* is a matrix whose entries are either 1 or -1. Two matrices A, B of the same order are said to be *D-similar* if there is a diagonal matrix D with diagonal entries equal to 1 or -1 such that $DAD = B$. We will need the following lemma.

LEMMA 6. *Let A be an $n \times n$ symmetric $\{\pm 1\}$-matrix with all diagonal entries equal to* 1. *Then either A is D-similar to J_n or A has a principal submatrix of order* 3 *which is similar to*

$$B_1 = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}.$$

Proof. The cases $n = 1, 2$ are obvious. Use induction on n for $n \geq 3$. First let $n = 3$. If $A = J_3$, there is nothing to prove. Otherwise A has an off-diagonal entry equal to -1. Then there are the following possibilities of A:

$$B_1, \quad \begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix},$$

$$\begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}.$$

It is easy to check that each of these matrices satisfies the conclusion. Now consider $n \geq 4$ and suppose the lemma holds for matrices of order $n - 1$. Let

$$A = \begin{bmatrix} 1 & u^T \\ u & A_1 \end{bmatrix}.$$

If A_1 has a principal submatrix of order 3 which is similar to B_1, then so does A. Otherwise, by the assumption, A_1 is D-similar to J_{n-1}. So A is D-similar to

$$H = \begin{bmatrix} 1 & v^T \\ v & J_{n-1} \end{bmatrix} = (h_{ij}).$$

If each entry of v is 1 or each entry of v is -1, then H and hence A are D-similar to J_n. Otherwise we have $h_{1,p} = -1$, $h_{1,q} = 1$ or $h_{1,p} = 1$, $h_{1,q} = -1$ for some $1 < p < q$. In the first case $H[1, p, q] = B_1$. In the second case $H[1, p, q]$ is D-similar to B_1. Therefore in both cases A has a principal submatrix which is similar to B_1. □

Two matrices A, B of the same order are said to be *sign-permutation similar* if there exist a permutation matrix P and a diagonal matrix D with diagonal entries equal to 1 or -1 such that $DP^TAPD = B$. It is clear that sign-permutation similarity is an equivalence relation.

THEOREM 7. *Let $A \in S_n[-a, a]$ with $n \geq 2$ and $a > 0$. Then*

$$s(A) \leq \begin{cases} \sqrt{2}na & \text{if } n \text{ is even,} \\ \sqrt{2n^2 - 1}a & \text{if } n \text{ is odd.} \end{cases}$$

If n is even, equality holds if and only if A is sign-permutation similar to

$$a\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes J_{\frac{n}{2}}.$$

If n is odd, equality holds if and only if A is sign-permutation similar to

$$\pm a\begin{bmatrix} J_{\frac{n+1}{2}} & J_{\frac{n+1}{2},\frac{n-1}{2}} \\ J_{\frac{n-1}{2},\frac{n+1}{2}} & -J_{\frac{n-1}{2}} \end{bmatrix}.$$

Proof. By considering $a^{-1}A$ instead of A, it suffices to prove the theorem for the case $a = 1$. Suppose $A \in S_n[-1, 1]$. Throughout this proof we write λ_j for $\lambda_j(A)$. For $x \in \mathbb{R}^n$, we always write its components as $x_1, \dots, x_n$. Given $A \in S_n[-1, 1]$, let $x, y \in \mathbb{R}^n$ be unit eigenvectors such that $\lambda_1 = x^T Ax$, $\lambda_n = y^T Ay$. Then

$$s(A) = x^T Ax - y^T Ay = e^T[A \circ (xx^T - yy^T)]e. \tag{9}$$

Note that the (i, j) entry of $xx^T - yy^T$ is $x_i x_j - y_i y_j$. We define a new matrix $\tilde{A} = (\tilde{a}_{ij})$ as $\tilde{a}_{ij} = 1$ if $x_i x_j - y_i y_j \geq 0$ and $\tilde{a}_{ij} = -1$ if $x_i x_j - y_i y_j < 0$. Then from (9) we have

$$\begin{aligned} s(A) &\leq x^T \tilde{A}x - y^T \tilde{A}y \\ &\leq \max\{w^T \tilde{A}w : \|w\| = 1, w \in \mathbb{R}^n\} - \min\{z^T \tilde{A}z : \|z\| = 1, z \in \mathbb{R}^n\} \\ &= s(\tilde{A}). \end{aligned}$$

Therefore the maximal spread can always be attained at some $\{\pm 1\}$-matrix. If $n = 2$, the conclusions of the theorem are easily checked to be true. Next we assume $n \geq 3$. Now suppose A is a $\{\pm 1\}$-matrix of order n.

The following three matrices will play a role in our proof:

$$B_1 = \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & -1 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix}.$$

Their eigenvalues are

$$\lambda(B_1) = \{2, 2, -1\}, \quad \lambda(B_2) = \{2, 1, -2\}, \quad \lambda(B_3) = \{2, -1, -2\}.$$

If A has a principal submatrix of order 3 which is similar to B_1, then by Lemma 3 $\lambda_2 \geq 2$. If A has a principal submatrix of order 3 which is similar to B_2, then by Lemma 3 $\lambda_2 \geq 1$. If A has a principal submatrix of order 3 which is similar to B_3, then by Lemma 3 $\lambda_{n-1} \leq -1$. In all three cases we have

$$\lambda_1^2 + \lambda_n^2 = \|A\|_F^2 - \sum_{j=2}^{n-1} \lambda_j^2 \leq n^2 - 1.$$

Hence

$$s(A) = \lambda_1 - \lambda_n \leq \sqrt{2(\lambda_1^2 + \lambda_n^2)} \leq \sqrt{2(n^2 - 1)} < \min\left\{\sqrt{2}n, \sqrt{2n^2 - 1}\right\}. \tag{10}$$

Thus if one of the above cases occurs, the spread is less than our claimed upper bound.

If all the diagonal entries of A are 1, then by Lemma 6 either A is D-similar to J_n or A has a principal submatrix of order 3 which is similar to B_1. Since $s(J_n) = n$, in both cases $s(A)$ is not the maximal value. If all the diagonal entries of A are -1, then since $s(-A) = s(A)$, this case is the same as what we just discussed.

Next consider those $\{\pm 1\}$-matrices A whose diagonal contains both 1 and -1. By simultaneous row and column permutations if necessary, we may suppose

$$A = \begin{bmatrix} A_r & A_{r,s} \\ A_{r,s}^T & A_s \end{bmatrix},$$

where A_r is of order r $(1 \le r \le n-1)$ and A_r's diagonal entries are all 1, and A_s is of order $s = n - r$ and A_s's diagonal entries are all -1. Since $s(-A) = s(A)$, we need consider only the case $r \ge s$. Then $r \ge 2$. By Lemma 6, either A_r is D-similar to J_r or A_r has a principal submatrix of order 3 which is similar to B_1. In the first case A is D-similar to a matrix whose rth leading principal submatrix is J_r, while in the second case $s(A)$ is not the maximal value. Thus we may suppose $A_r = J_r$. Now two cases can occur. (i) $A_{r,s}$ has a column which contains both 1 and -1. Then A has a principal submatrix which is similar to B_2, and $s(A)$ is not the maximal value. (ii) Each column of $A_{r,s}$ contains only 1 or only -1. Then A is D-similar to

$$G = \begin{bmatrix} J_r & J_{r,s} \\ J_{s,r} & \tilde{A}_s \end{bmatrix},$$

where all the diagonal entries of $\tilde{A}_s$ remain -1. If $\tilde{A}_s$ has an off-diagonal entry equal to 1, then G has B_3 as a principal submatrix and $s(G)$ is not the maximal value. Thus we further consider the case $\tilde{A}_s = -J_s$.

Now there remains the case

$$A = \begin{bmatrix} J_r & J_{r,s} \\ J_{s,r} & -J_s \end{bmatrix}, \tag{11}$$

where $r \ge s$. It is easy to see that

$$s\left(\begin{bmatrix} J_r & J_{r,s} \\ J_{s,r} & -J_s \end{bmatrix}\right) = \sqrt{2n^2 - (2r-n)^2}. \tag{12}$$

Therefore by (12) the maximal spread of the matrices in (11) is $\sqrt{2}n$ attained uniquely at $r = n/2$ if n is even, and the maximal spread is $\sqrt{2n^2-1}$ attained uniquely at $r = (n+1)/2$ if n is odd. For the odd case note that we have assumed $r \ge s = n - r$, and hence $r = (n-1)/2$ does not occur. At this stage we have found the maximal spread of $A \in S_n[-1, 1]$.

Next we determine those matrices which attain the maximal spread. Suppose $A \in S_n[-1, 1]$ attains the maximal spread and x, y are the unit eigenvectors corresponding to λ_1 and λ_n, respectively. Assume that $xx^T - yy^T$ has a zero entry, say, $x_i x_j - y_i y_j = 0$ for some i, j. From (9) it is clear that we can change the corresponding entry a_{ij} of A arbitrarily without affecting the value of $s(A)$. So we may suppose $a_{ij} = 0$. Then

$$n^2 - 1 \ge \|A\|_F^2 \ge \lambda_1^2 + \lambda_n^2 \ge \frac{(\lambda_1 - \lambda_n)^2}{2} = \begin{cases} n^2 & \text{if } n \text{ is even,} \\ n^2 - \frac{1}{2} & \text{if } n \text{ is odd,} \end{cases}$$

which is a contradiction. Thus every entry of $xx^T - yy^T$ is nonzero. By (9) we deduce that A must be a $\{\pm 1\}$-matrix. On the other hand, the above analysis leading to the maximal spread shows that when n is even, $s(A) = \sqrt{2}n$ if and only if A is sign-permutation similar to

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes J_{\frac{n}{2}},$$

and when n is odd, $s(A) = \sqrt{2n^2 - 1}$ if and only if A is sign-permutation similar to

$$\pm \begin{bmatrix} J_{\frac{n+1}{2}} & J_{\frac{n+1}{2},\frac{n-1}{2}} \\ J_{\frac{n-1}{2},\frac{n+1}{2}} & -J_{\frac{n-1}{2}} \end{bmatrix}.$$

The permutation similarity comes from our operation to put positive diagonal entries together and let them appear first. The possible minus sign comes from the fact that $s(-A) = s(A)$, which we used to simplify our analysis. Note also that in the case when n is even,

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes J_{\frac{n}{2}} \quad \text{and} \quad -\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes J_{\frac{n}{2}}$$

are sign-permutation similar, and the minus sign need not appear in our assertion for the equality case. This completes the proof. ◻

Let $e_t \in \mathbb{R}^t$ denote the all-one vector. By Theorem 7 and (9) we get the following interesting corollary.

COROLLARY 8.

$$\max\left\{\sum_{i,j=1}^{n} |x_i x_j - y_i y_j| : \|x\| = \|y\| = 1, x, y \in \mathbb{R}^n\right\} = \begin{cases} \sqrt{2}n & \text{if } n \text{ is even,} \\ \sqrt{2n^2-1} & \text{if } n \text{ is odd.} \end{cases}$$

The maximum is attained at x, y if and only if $x = DPx_0$, $y = DPy_0$ for some diagonal matrix D with diagonal entries equal to 1 or -1 and some permutation matrix P where

$$x_0 = \begin{pmatrix} ae_{n/2} \\ be_{n/2} \end{pmatrix}, \quad y_0 = \begin{pmatrix} -be_{n/2} \\ ae_{n/2} \end{pmatrix}, \quad a = (1+\sqrt{2})b, \quad b = \frac{1}{\sqrt{(2+\sqrt{2})n}}$$

if n is even and

$$x_0 = \begin{pmatrix} ae_{(n+1)/2} \\ be_{(n-1)/2} \end{pmatrix}, a = \sqrt{\frac{1}{n+1}\left(1 + \frac{n}{\sqrt{2n^2-1}}\right)}, b = \sqrt{\frac{1}{n-1}\left(1 - \frac{n}{\sqrt{2n^2-1}}\right)}$$

$$y_0 = \begin{pmatrix} ce_{(n+1)/2} \\ de_{(n-1)/2} \end{pmatrix}, c = \sqrt{\frac{1}{n+1}\left(1 - \frac{n}{\sqrt{2n^2-1}}\right)}, d = -\sqrt{\frac{1}{n-1}\left(1 + \frac{n}{\sqrt{2n^2-1}}\right)}$$

if n is odd.

We remark that the above x_0 and y_0 are the unit eigenvectors corresponding to the largest and smallest eigenvalues of the maximizing matrix in Theorem 7.

We have the following two obvious problems which are not solved here.

Problem 1. For a given integer j with $2 \le j \le n-1$, determine

$$\max\{\lambda_j(A) : A \in S_n[a,b]\},$$

$$\min\{\lambda_j(A) : A \in S_n[a,b]\}$$

and determine which matrices attain the maximum and which matrices attain the minimum.

Problem 2. For generic $a < b$, determine

$$\max\{s(A) : A \in S_n[a, b]\},$$

where $s(A)$ denotes the spread of A, and determine which matrices attain the maximum.

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