arXiv:1401.7084v7 [math.NA] 27 Mar 2014

Bounds on determinants of perturbed diagonal matrices

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March 28, 2014

Abstract

We give upper and lower bounds on the determinant of a perturbation of the identity matrix or, more generally, a perturbation of a nonsingular diagonal matrix. The matrices considered are, in general, diagonally dominant. The lower bounds are best possible, and in several cases they are stronger than well-known bounds due to Ostrowski and other authors. If $A = I - E$ is a real $n \times n$ matrix and the elements of E are bounded in absolute value by $\varepsilon \le 1/n$, then a lower bound of Ostrowski (1938) is $\det(A) \ge 1 - n\varepsilon$. We show that if, in addition, the diagonal elements of E are zero, then a best-possible lower bound is

$$\det(A) \ge (1 - (n-1)\varepsilon)\,(1+\varepsilon)^{n-1}.$$

Corresponding upper bounds are respectively

$$\det(A) \le (1 + 2\varepsilon + n\varepsilon^2)^{n/2}$$

and

$$\det(A) \le (1 + (n-1)\varepsilon^2)^{n/2}.$$

The first upper bound is stronger than Ostrowski's bound (for $\varepsilon < 1/n$) $\det(A) \le (1 - n\varepsilon)^{-1}$. The second upper bound generalises Hadamard's inequality, which is the case $\varepsilon = 1$. A necessary and sufficient condition for our upper bounds to be best possible for matrices of order n and all positive ε is the existence of a skew-Hadamard matrix of order n.

1 Introduction

Many bounds on determinants of diagonally dominant matrices A have been given in the literature. See, for example, Muir [24], Ostrowski [32], Price [34], and more recently Bhatia and Jain [2], Elsner [11], Horn and Johnson [18], Ipsen and Rehman [19], Li and Chen [21], and the references given there.

Except in Theorem 1, we restrict attention to the case that we have uniform upper bounds $|a_{ij}| \le \varepsilon$ on the sizes of the off-diagonal entries a_{ij} $(i \ne j)$ of A. Since the nonzero diagonal elements a_{ii} of A can be assumed to be 1 (or close to 1) by row or column scaling, we assume that $a_{ii} = 1$ or $|a_{ii} - 1| \le \delta$, where δ is a small parameter, possibly different from ε. In Corollary 1 we relax the condition on a_{ii} to a one-sided constraint $a_{ii} \ge 1-\delta$. The results have applications to proofs of lower bounds for the Hadamard maximal determinant problem; this was our original motivation (see [4, 5]). Regarding other reasons for considering bounds on determinants, we refer to Bornemann [3, footnote 4].

For purposes of comparison with our bounds, we first state some known bounds. For a square matrix $A = (a_{ij})$ of order n, define

$$h_i := |a_{ii}| - \sum_{j \ne i} |a_{ij}| = 2|a_{ii}| - \sum_{j=1}^{n} |a_{ij}| \ \text{ for } \ 1 \le i \le n,$$

and assume that the h_i are positive. It is well-known that $\det(A) \ne 0$; see Taussky [37] for the history of this theorem. Ostrowski [27] showed that

$$|\det(A)| \ge h_1 h_2 \cdots h_n. \tag{1}$$

If we assume that $\operatorname{diag}(A) = I$ and that the off-diagonal elements of A satisfy $|a_{ij}| \le \varepsilon$ $(i \ne j)$, where $(n-1)\varepsilon < 1$, then Ostrowski's bound (1) reduces to

$$\det(A) \ge (1 - (n-1)\varepsilon)^n. \tag{2}$$

The same bound follows from Gerschgorin's theorem [15, 38]. Observe that the right side of (2) is $1 - n(n-1)\varepsilon + O(\varepsilon^2)$, so the perturbation appears to be of order ε. As pointed out by Ostrowski [28, 30, 31], the perturbation is actually of order ε^2, so the bound (2) is weak, at least for small ε. Similar remarks apply to the inequalities of Oeder [25] and Price [34]. An improved lower bound given by Ostrowski [28, Satz VI] reduces (under the same assumptions on A) to

$$\det(A) \ge \left(1 - (n-1)^2\varepsilon^2\right)^{\lfloor n/2 \rfloor}. \tag{3}$$

Ostrowski [28, Satz VI] also gives an upper bound, which reduces to

$$\det(A) \le \left(1 + (n-1)^2\varepsilon^2\right)^{\lfloor n/2 \rfloor}. \tag{4}$$

In both these bounds the perturbation is clearly of order ε^2, as expected from consideration of the case $n = 2$, where $1 - \varepsilon^2 \le \det(A) \le 1 + \varepsilon^2$.

A different lower bound, due to von Koch [20] (see Ostrowski [27, §2]), reduces under the same assumptions to

$$\det(A) \ge e^{n(n-1)\varepsilon}(1 - (n-1)\varepsilon)^n. \tag{5}$$

For $n > 1$ the inequality (5) is clearly stronger than (2), but a computation shows that it is weaker than (3) under our assumptions.

Suppose we allow a perturbation of the diagonal elements, so $A = I - E$ where $|e_{ij}| \le \varepsilon < 1/n$, $1 \le i, j \le n$. A pair of bounds given by Ostrowski in [29, eqn. (5,5)] is, in our notation,

$$\det(A) \ge 1 - n\varepsilon \tag{6}$$

and

$$\det(A) \le \frac{1}{1 - n\varepsilon} \cdot \tag{7}$$

In §3 we consider lower bounds on $\det(A)$, where A is a matrix of the form $I - E$, and the elements of E are small in some sense. In Theorem 1 a matrix F of non-negative elements f_{ij} is given, and $|e_{ij}| \le f_{ij}$. The theorem gives a lower bound $\det(I-F)$ on $\det(A)$ under the condition that $\rho(F) \le 1$, where $\rho(\cdot)$ denotes the spectral radius.[1] Theorem 1 is similar to [18, Thm. 2.5.4(c)], but less restrictive as the e_{ij} may be positive or negative.[2]

Corollary 1 gives a best-possible lower bound on $\det(A)$ when the diagonal elements of E satisfy $e_{ii} \le \delta$ (only a one-sided constraint is necessary) and the off-diagonal elements satisfy $|e_{ij}| \le \varepsilon$, assuming that $\delta + (n-1)\varepsilon \le 1$. Corollaries 2 and 3 give lower bounds that are special cases of Corollary 1. Corollary 2 is equivalent to Ostrowski's lower bound (6), but our other lower-bound results appear to be new. Corollary 3 is much stronger than the bound (2), and also slightly stronger than Ostrowski's improved bound (3) if $n > 2$.

In Theorem 2 we deduce (from Corollary 3) a lower bound on $\det(A)$ when the condition $|a_{ij}| \le \varepsilon |a_{ii}|$ holds for all off-diagonal elements a_{ij}, and $(n-1)\varepsilon \le 1$. Similar remarks apply to Theorem 2 as to Corollary 3.

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[1] Thus $I - F$ is a (possibly singular) M-matrix, but A is not necessarily a Z-matrix.

[2] Theorem 1 is close to the (real case of) [18, problem 2.5.31(d)]. Our proof is similar to the sketch given in [18, problem 2.5.30].

In §4 we consider upper bounds on $\det(A)$ when the elements of $E = I - A$ are (usually) small. Upper bounds when A is close to a diagonal matrix follow by row or column scaling, as in the proof of Theorem 2. Theorem 3 assumes that $|e_{ij}| \le \varepsilon$ and gives two upper bounds, the second applying under the extra condition that $\mathrm{diag}(E) = 0$. In the case $\varepsilon = 1$, the second bound (9) reduces to Hadamard's upper bound $n^{n/2}$ for the determinants of $\{\pm 1\}$-matrices. For $\varepsilon > 0$, our first upper bound (8) is always stronger than Ostrowski's upper bound (7). Our second upper bound (9) is stronger than Ostrowski's upper bound (4) if $n > 2$ and $(n-1)\varepsilon < 1$ (this condition on ε is necessary for the validity of (4), but is not required for (9)).

To summarise, we can not improve on Ostrowski's inequality (6) as it is best-possible, but we do improve on the inequalities (2)–(5) and (7).

As shown in Theorem 4, the upper bounds of Theorem 3 are best possible for matrices of order n if and only if there exists a skew-Hadamard matrix of order n. This condition is known to hold for $n = 1, 2$, and all multiples of four up to and including 4×68, as well as infinitely many larger n, such as all powers of two, see [9, 10, 14, 35].

Remark 5 gives attainable determinants that are close to the upper bounds of Theorem 3. These are of interest when n is not the order of a skew-Hadamard matrix, since in such cases the bounds of Theorem 3 are not best-possible, and the best-possible bounds are only known for a few small orders.

In §4.1 we consider some small orders n. The limited evidence suggests that the behaviour depends on the congruence class $n \bmod 4$. This is not surprising, as it also appears to be true for the (related) Hadamard maximal determinant problem [26].

Via the transformation $\varepsilon \mapsto 1/x$, we easily obtain upper-bound results for matrices whose off-diagonal entries are in $[-1, 1]$ and whose diagonal elements are all equal to a real parameter x.

In the case $\varepsilon = 1$, our upper-bound results are related to results on $\{\pm 1\}$-matrices of skew-symmetric type [1], conference matrices [6], Cameron's "hot" and "cold" matrices [7], and the Hadamard maximal determinant problem [26]. Thus, our upper-bound results may be regarded as generalising some known results on $\{0, \pm 1\}$-matrices by incorporating a parameter ε (or $x = 1/\varepsilon$).

2 Notation and definitions

All our matrices are square. The *order* of such a matrix is the number of rows (or columns) of the matrix. $\mathbb{R}^{n \times n}$ is the set of all $n \times n$ real matrices.

Matrices are denoted by capital letters A etc, and their elements by the corresponding lower-case letters, e.g. $a_{i,j}$ or simply a_{ij} if the meaning is clear.

The eigenvalues of a (square) matrix A of order n are written as $\lambda_i(A)$, $1 \le i \le n$. We define the *trace* $\mathrm{Tr}(A) := \sum_{1\le i\le n} a_{ii}$. It is well-known that $\mathrm{Tr}(A) = \sum_{1\le i\le n} \lambda_i(A)$.

$\rho(A) := \max_{1\le i\le n} |\lambda_i(A)|$ denotes the *spectral radius* of a matrix A.

The identity matrix of order n is denoted by I_n, or simply by I if the order is clear from the context. The matrix of all ones is J (or J_n), so $J = ee^T$, where e is the (column) n-vector of all ones.

U_n denotes the strictly upper triangular $n \times n$ matrix defined by

$$u_{ij} = \begin{cases} 1 \text{ if } i < j; \\ 0 \text{ otherwise.} \end{cases}$$

A *skew-Hadamard matrix* is a Hadamard matrix H satisfying the condition $H + H^T = 2I$. An equivalent condition is that $H - I$ is a skew-symmetric matrix.

Finally, δ and ε are non-negative parameters, subject to certain size restrictions that are specified as needed.

3 Lower bounds

In this section we give lower bounds on the determinant of a matrix that is close to the identity matrix or, in the case of Theorem 2, close to a diagonal matrix. We start with a general theorem and then deduce some corollaries that are useful in applications. The proof of Theorem 1 uses the Fredholm determinant formula[3] in a manner similar to the proof of (6) given in [29].

Theorem 1. *Let $F \in \mathbb{R}^{n\times n}$, $f_{ij} \ge 0$, $\rho(F) \le 1$. If $A = I - E \in \mathbb{R}^{n\times n}$, where $|e_{ij}| \le f_{ij}$, then*

$$\det(A) \ge \det(I - F).$$

Proof. First suppose that $\rho(F) < 1$. By Gelfand's formula for the spectral radius of a matrix [13],

$$\rho(E) = \lim_{k\to\infty} ||E^k||_2^{1/k} \le \lim_{k\to\infty} ||F^k||_2^{1/k} = \rho(F) < 1,$$

[3] Fredholm [12], see also Bornemann [3, eqn. (3.3)], von Koch [20] and Plemelj [33].

so the series

$$\sum_{k=1}^{\infty} \frac{1}{k} E^k$$

converges. Hence, by the Fredholm determinant formula

$$\det(A) = \exp\left(-\mathrm{Tr}\left(\sum_{k=1}^{\infty} \frac{1}{k} E^k\right)\right) = \exp\left(-\sum_{k=1}^{\infty} \frac{1}{k} \mathrm{Tr}(E^k)\right).$$

The entries in E^k are polynomials in the e_{ij} with non-negative coefficients; hence they take their maximum values when $E = F$. The result (still under the assumption that $\rho(F) < 1$) follows from the monotonicity of the exponential function.

To deal with the case $\rho(F) = 1$ we may choose any $x \in (0, 1)$ and replace E by xE and F by xF in the above argument, showing that

$$\det(I - xE) \geq \det(I - xF).$$

Now let $x \to 1$ and use continuity of the determinant. □

Remark 1. For $n > 1$, it is not possible to weaken the condition $\rho(F) \leq 1$ in Theorem 1. For even n, this is shown by the counter-example $E = I$, $F = \phi I$, where $\phi > 1$. Counter-examples for odd $n > 1$ are also easy to construct using diagonal matrices E and F.

Lemma 1. *Let $A = I - E \in \mathbb{R}^{n \times n}$, where $|e_{ij}| \leq \varepsilon$ for $i \neq j$, $|e_{ii}| \leq \delta$ for $1 \leq i \leq n$, and $\delta + (n-1)\varepsilon \leq 1$. Then*

$$\det(A) \geq (1 - \delta - (n-1)\varepsilon)(1 - \delta + \varepsilon)^{n-1},$$

and the inequality is sharp.

Proof. The result is immediate if $n = 1$, so suppose that $n \geq 2$. Define $F := (\delta - \varepsilon)I + \varepsilon J$, so F is a Toeplitz matrix with diagonal entries δ and off-diagonal entries ε.

Observe that $Je = ne$, so J has an eigenvalue $\lambda_1(J) = n$; the other $n - 1$ eigenvalues are zero since J has rank 1.

Since εJ has one eigenvalue equal to $n\varepsilon$ and $n - 1$ eigenvalues equal to zero, it is immediate that F has eigenvalues $\delta - \varepsilon + n\varepsilon = \delta + (n-1)\varepsilon$ and $\delta - \varepsilon$. Thus

$$\rho(F) = \max(\delta + (n-1)\varepsilon, |\delta - \varepsilon|) = \delta + (n-1)\varepsilon \leq 1.$$

Also, the eigenvalues of $I - F$ are $1 - \delta - (n-1)\varepsilon$ with multiplicity 1, and $1 - \delta + \varepsilon$ with multiplicity $n - 1$, so

$$\det(I - F) = (1 - \delta - (n-1)\varepsilon)\,(1 - \delta + \varepsilon)^{n-1}\,.$$

Thus, the inequality follows from Theorem 1. It is sharp because equality holds for $A = I - F$. $\square$

Corollary 1 is similar to Lemma 1, but the condition on e_{ii} is one-sided. This is useful in applications of the probabilistic method using one-sided inequalities such as Cantelli's inequality [8], see for example [5, Thms. 4–5].

Corollary 1. *Let $A = I - E \in \mathbb{R}^{n\times n}$, where $|e_{ij}| \le \varepsilon$ for $i \ne j$ and $e_{ii} \le \delta$ for $1 \le i \le n$. If $0 \le \delta \le 1 - (n-1)\varepsilon$, then*

$$\det(A) \ge (1 - \delta - (n-1)\varepsilon)(1 - \delta + \varepsilon)^{n-1}\,,$$

and the inequality is sharp.

Proof. We deduce the result from Lemma 1 using "diagonal scaling". Let $D \in \mathbb{R}^{n\times n}$ be the diagonal matrix with diagonal elements $d_i = \max(1, a_{ii})$. Note that $d_i \ge 1$, so $D^{-1} = \mathrm{diag}(d_i^{-1})$ is well-defined. Define $A' = D^{-1}A$ and $E' = I - A'$. Since $a'_{ij} = d_i^{-1}a_{ij}$, we have $|e'_{ij}| = |d_i^{-1}e_{ij}| \le |e_{ij}| \le \varepsilon$ for $i \ne j$, and

$$e'_{ii} = \begin{cases} e_{ii} \text{ if } e_{ii} \ge 0, \\ 0 \text{ if } e_{ii} < 0, \end{cases}$$

so $0 \le e'_{ii} \le \delta$. Thus, we can apply Lemma 1 to $A' = I - E'$, giving

$$\det(A') \ge (1 - \delta - (n-1)\varepsilon)(1 - \delta + \varepsilon)^{n-1} \ge 0.$$

Since $\det(A) = \det(D)\det(A') \ge \det(A')$, the inequality follows. It is sharp because equality holds if we take $A = I - F$, where F is as in the proof of Lemma 1. $\square$

Corollaries 2–3 are simple consequences of Lemma 1. They are stated in [4, Lemmas 8–9], but only Corollary 2 is proved there. Corollary 2 follows from Ostrowski's lower bound (6), although Ostrowski did not explicitly state that the lower bound is sharp, perhaps because the corresponding upper bound (7) is not sharp (see Remark 4).

Corollary 2. *If $A = I - E \in \mathbb{R}^{n\times n}$, $|e_{ij}| \le \varepsilon$ for $1 \le i, j \le n$, and $n\varepsilon \le 1$, then*

$$\det(A) \ge 1 - n\varepsilon,$$

and the inequality is sharp.

Proof. This is the case $\delta = \varepsilon$ of Lemma 1. Equality occurs when $E = \varepsilon J$. $\square$

Corollary 3 is sharper than Ostrowski's bound (3) if $n > 2$ (they are the same if $n \le 2$). Corollary 3 is also sharper than von Koch's bound (5). This is perhaps surprising, since the proofs of both results depend (directly or indirectly) on Fredholm's determinant formula.

Corollary 3. *If $A = I - E \in \mathbb{R}^{n\times n}$, $|e_{ij}| \le \varepsilon$ for $1 \le i,j \le n$, $e_{ii} = 0$ for $1 \le i \le n$, and $(n-1)\varepsilon \le 1$, then*

$$\det(A) \ge (1 - (n-1)\varepsilon)\ (1+\varepsilon)^{n-1},$$

and the inequality is sharp.

Proof. This is the case $\delta = 0$ of Lemma 1. Equality occurs when $E = \varepsilon(J - I)$. $\square$

The results presented so far apply to perturbations of the identity matrix. To bound the determinant of a perturbed diagonal matrix A, we can first multiply it by a diagonal matrix approximating A^{-1}. Theorem 2 uses this "preconditioning" idea to give a lower bound on the determinant of a diagonally dominant matrix. A similar idea was used in the proof of Corollary 1 above.

Theorem 2. *If $A \in \mathbb{R}^{n\times n}$ satisfies $|a_{ij}| \le \varepsilon |a_{ii}|$ for all $i \ne j$, $1 \le i,j \le n$, then*

$$|\det(A)| \ge \left(\prod_{i=1}^{n} |a_{ii}|\right) (1 - (n-1)\varepsilon)\,(1+\varepsilon)^{n-1}.$$

Remark 2. The simpler but slightly weaker inequality

$$|\det(A)| \ge \left(\prod_{i=1}^{n} |a_{ii}|\right) \left(1 - (n-1)^2\varepsilon^2\right)$$

follows easily, since

$$(1 - (n-1)\varepsilon)\,(1+\varepsilon)^{n-1} \ge (1 - (n-1)\varepsilon)\,(1 + (n-1)\varepsilon) = 1 - (n-1)^2\varepsilon^2.$$

Proof of Theorem 2. If $(n-1)\varepsilon \ge 1$ then the inequality is trivial as the right side is not positive. Hence, assume that $0 \le (n-1)\varepsilon < 1$. If any $a_{ii} = 0$ then the result is trivial. Otherwise, apply Corollary 3 to SA, where $S = \mathrm{diag}(a_{ii}^{-1})$. Since $\det(A) = \det(SA)\prod_i a_{ii}$, the result follows. $\square$

Remark 3. The bound of Theorem 2 is much stronger than the bound

$$|\det(A)| \ge \left(\prod_{i=1}^{n} |a_{ii}|\right)(1-(n-1)\varepsilon)^n$$

that follows from Gerschgorin's theorem or Ostrowski's inequality (1). For example, if $a_{ii} = 1$ for $1 \le i \le n$ and $(n-1)\varepsilon = 1/2$, then Theorem 2 gives the lower bound $3/4$, whereas Gerschgorin's theorem and Ostrowski's inequality (2) both give 2^{-n}. Theorem 2 is stronger than Ostrowski's improved lower bound (3) if $n > 2$; the bound given in Remark 2 is stronger than (3) if $n > 3$.

To illustrate the lower bounds that apply when $\operatorname{diag}(A) = I$, suppose that $n = 5$ and $\varepsilon = 1/8$. Then Gerschgorin/Ostrowski (2) gives the lower bound $2^{-5} = 0.03125$, von Koch (5) gives $e^{5/2}/2^5 \approx 0.3807$, Ostrowski (3) gives $9/16 = 0.5625$, Remark 2 gives $3/4 = 0.75$, Corollary 3 and Theorem 2 give $3^8/2^{13} \approx 0.8009$.

4 Upper bounds

In this section we give upper bounds on $\det(A)$ to complement the lower bounds of §3. Theorem 3 gives upper bounds analogous to the lower bounds in Corollaries 2–3. The upper bounds in Theorem 3 follow easily from the classical Hadamard bound [16, 17, 22]. Given n, we may ask for which ε the inequalities of Theorem 3 are attainable. This question is closely related to the question of existence of a skew-Hadamard matrix of order n, as shown by Theorem 4. Before proving Theorem 4, we consider some small examples to illustrate how the optimal upper bound depends on arithmetic properties of the order n (unlike the optimal lower bound).

Theorem 3. *If $A = I - E \in \mathbb{R}^{n\times n}$, $|e_{ij}| \le \varepsilon$ for $1 \le i, j \le n$, then*

$$\det(A) \le (1 + 2\varepsilon + n\varepsilon^2)^{n/2}. \tag{8}$$

If, in addition, $e_{ii} = 0$ for $1 \le i \le n$, then

$$\det(A) \le (1 + (n-1)\varepsilon^2)^{n/2}. \tag{9}$$

Proof. Let the columns of A be $u_1, u_2, \ldots, u_n$. From Hadamard's inequality,

$$\det(A) \le \prod_{i=1}^{n} ||u_i||_2 \,.$$

However, the condition $|e_{ij}| \le \varepsilon$ implies that

$$||u_i||_2^2 \le (1+\varepsilon)^2 + (n-1)\varepsilon^2 = 1 + 2\varepsilon + n\varepsilon^2.$$

Hence, the result (8) follows. The proof of (9) is similar. □

Remark 4. In view of Lemma 2 below, the inequality (8) of Theorem 3 is stronger than Ostrowski's upper bound (7) for all $n \ge 1$ and $\varepsilon > 0$. Hence, Ostrowski's upper bound (7) is never sharp. Note that Theorem 3 applies for all $\varepsilon \ge 0$; there is no need for a restriction such as $n\varepsilon < 1$.

The upper bound (9) reduces to the Hadamard bound $n^{n/2}$ if $\varepsilon = 1$. We find that (9) is stronger than (4) if $n > 2$, and equal if $n \le 2$, assuming that $(n-1)\varepsilon \le 1$ since this is necessary for the proof of (4). For example, if $n = 5$ and $\varepsilon = 1/8$, then (9) gives the upper bound $(17/16)^{5/2} \approx 1.16365$, and (4) gives $25/16 = 1.5625$. The best possible upper bound is $1 + 10\varepsilon^2 + 21\varepsilon^4 \approx 1.16138$ (see §4.1).

Lemma 2. *If* $n \ge 1$, $\varepsilon > 0$, *and* $n\varepsilon < 1$, *then*

$$\left(1 + 2\varepsilon + n\varepsilon^2\right)^{n/2} < \frac{1}{1 - n\varepsilon} \cdot$$

Proof. It is sufficient to show that

$$1 + 2\varepsilon + n\varepsilon^2 < (1 - n\varepsilon)^{-2/n}.$$

Expanding the right-hand side as a power series in ε, we obtain

$$(1 - n\varepsilon)^{-2/n} = 1 + 2\varepsilon + (n+2)\varepsilon^2 + \sum_{k=3}^{\infty} \alpha_k(n)\varepsilon^k,$$

where the $\alpha_k(n)$ are polynomials in n, with non-negative coefficients. □

Remark 5. Some "large" determinants, generally smaller by $O(\varepsilon^4)$ than the corresponding upper bounds of Theorem 3, are

$$\det((1+\varepsilon)I_n + \varepsilon(U_n - U_n^T)) = \frac{(1+2\varepsilon)^n + 1}{2} \tag{10}$$

and

$$\det(I_n + \varepsilon(U_n - U_n^T)) = \frac{(1+\varepsilon)^n + (1-\varepsilon)^n}{2}\,, \tag{11}$$

corresponding to the upper bounds (8) and (9) respectively.[4] The upper-triangular matrix U_n is defined in §2.

[4] To prove (11), use row and column operations to transform the matrix to tridiagonal form, then prove the result by induction on n using the 3-term recurrence derived from the tridiagonal matrix. Equation (10) follows from (11) by a change of variables.

4.1 Small examples

We illustrate the inequalities (9) and (11) and give best-possible upper bounds for small orders n. Examples for the inequalities (8) and (10) may be derived by replacing ε by $\varepsilon/(1+\varepsilon)$.

Consider performing an exhaustive search for the maximal determinant (as a function of ε). For a naive search the size of the search space is $2^{n(n-1)}$. By using various symmetries we can assume that the signs in the first row are all plus, and that in the first column there are k plus signs followed by $n-k$ minus signs (for $1 \le k \le n$), so the search space size is reduced to $n\,2^{(n-1)(n-2)}$. An exhaustive search is feasible for $n \le 6$.

Order 2. The extreme cases are

$$\begin{vmatrix} 1 & \varepsilon \\ -\varepsilon & 1 \end{vmatrix} = \begin{vmatrix} 1 & -\varepsilon \\ \varepsilon & 1 \end{vmatrix} = 1 + \varepsilon^2. \tag{12}$$

Here (9) and (11) are both best possible for all $\varepsilon > 0$.

Order 3. An extreme case (not unique) for small ε is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon \\ -\varepsilon & 1 & \varepsilon \\ -\varepsilon & -\varepsilon & 1 \end{vmatrix} = 1+3\varepsilon^2 = \frac{(1+\varepsilon)^3 + (1-\varepsilon)^3}{2} < (1+2\varepsilon^2)^{3/2} = 1+3\varepsilon^2+O(\varepsilon^4).$$

Here (11) is best possible for $\varepsilon \in (0, 1]$, but (9) is not. Note that

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon \\ -\varepsilon & 1 & \varepsilon \\ \varepsilon & -\varepsilon & 1 \end{vmatrix} = 1 + \varepsilon^2 + 2\varepsilon^3 \tag{13}$$

is larger than $1+3\varepsilon^2$ when $\varepsilon > 1$. When $\varepsilon = 1$ we obtain (in both cases) the maximal determinant of 4 for 3×3 $\{\pm 1\}$-matrices [26].

Order 4. An extreme case is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon & \varepsilon \\ -\varepsilon & 1 & \varepsilon & -\varepsilon \\ -\varepsilon & -\varepsilon & 1 & \varepsilon \\ -\varepsilon & \varepsilon & -\varepsilon & 1 \end{vmatrix} = 1 + 6\varepsilon^2 + 9\varepsilon^4. \tag{14}$$

Here (9) is best possible, but (11) is not. Note that the matrix may be written as $(1-\varepsilon)I + \varepsilon H$, where H is a skew-Hadamard matrix. Similarly for $n = 1$ and $n = 2$. It follows that Theorem 3 is best possible for $n \in \{1, 2, 4\}$. This result is generalised in Theorem 4 below.

Order 5. There are four cases (15)–(18), found by an exhaustive search. For each interval $X = (0, 1/3)$, $(1/3, 3/5)$, $(3/5, 1)$, $(1, \infty)$, there is a unique polynomial that gives the maximal determinant for all $\varepsilon \in X$. The matrices that give each polynomial are not unique. We give one example for each interval.

For $\varepsilon \in [0, 1/3]$, the maximal determinant is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon & \varepsilon & \varepsilon \\ -\varepsilon & 1 & \varepsilon & -\varepsilon & \varepsilon \\ -\varepsilon & -\varepsilon & 1 & \varepsilon & \varepsilon \\ -\varepsilon & \varepsilon & -\varepsilon & 1 & -\varepsilon \\ -\varepsilon & -\varepsilon & -\varepsilon & \varepsilon & 1 \end{vmatrix} = 1 + 10\varepsilon^2 + 21\varepsilon^4, \tag{15}$$

lying between the attainable bound (11) of $1 + 10\varepsilon^2 + 5\varepsilon^4$ and the upper bound (9) of $1 + 10\varepsilon^2 + 30\varepsilon^4 + O(\varepsilon^6)$.

When $\varepsilon \in (1/3, 3/5]$, a larger determinant is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon & \varepsilon & \varepsilon \\ -\varepsilon & 1 & \varepsilon & -\varepsilon & \varepsilon \\ -\varepsilon & -\varepsilon & 1 & \varepsilon & \varepsilon \\ -\varepsilon & \varepsilon & -\varepsilon & 1 & \varepsilon \\ \varepsilon & -\varepsilon & -\varepsilon & -\varepsilon & 1 \end{vmatrix} = 1 + 8\varepsilon^2 + 6\varepsilon^3 + 15\varepsilon^4 + 18\varepsilon^5. \tag{16}$$

The matrices in (15)–(16) can be obtained by adding a border of one row and column to the matrix given above for order 4.

When $\varepsilon \in (3/5, 1]$, a larger determinant is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon & \varepsilon & \varepsilon \\ -\varepsilon & 1 & -\varepsilon & \varepsilon & -\varepsilon \\ -\varepsilon & -\varepsilon & 1 & \varepsilon & -\varepsilon \\ \varepsilon & -\varepsilon & -\varepsilon & 1 & -\varepsilon \\ -\varepsilon & -\varepsilon & -\varepsilon & \varepsilon & 1 \end{vmatrix} = 1 + 2\varepsilon^2 + 16\varepsilon^3 + 21\varepsilon^4 + 8\varepsilon^5. \tag{17}$$

When $\varepsilon > 1$, a larger determinant is given by the circulant

$$\begin{vmatrix} 1 & \varepsilon & -\varepsilon & \varepsilon & \varepsilon \\ \varepsilon & 1 & \varepsilon & -\varepsilon & \varepsilon \\ \varepsilon & \varepsilon & 1 & \varepsilon & -\varepsilon \\ -\varepsilon & \varepsilon & \varepsilon & 1 & \varepsilon \\ \varepsilon & -\varepsilon & \varepsilon & \varepsilon & 1 \end{vmatrix} = 1 + 10\varepsilon^3 + 15\varepsilon^4 + 22\varepsilon^5. \tag{18}$$

When $\varepsilon = 1$, the three cases (16)–(18) all give the maximal determinant 48 for 5×5 $\{\pm 1\}$-matrices, see [23, 26].

Order 6. There are three cases (19)–(21), found by an exhaustive search. For $\varepsilon \in [0, \varepsilon_1]$, where $\varepsilon_1 \approx 0.3437$, the maximal determinant is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon & \varepsilon & \varepsilon & \varepsilon \\ -\varepsilon & 1 & \varepsilon & \varepsilon & \varepsilon & -\varepsilon \\ -\varepsilon & -\varepsilon & 1 & \varepsilon & -\varepsilon & \varepsilon \\ -\varepsilon & -\varepsilon & -\varepsilon & 1 & \varepsilon & \varepsilon \\ -\varepsilon & -\varepsilon & \varepsilon & -\varepsilon & 1 & \varepsilon \\ -\varepsilon & \varepsilon & -\varepsilon & -\varepsilon & -\varepsilon & 1 \end{vmatrix} = 1 + 15\varepsilon^2 + 63\varepsilon^4 + 81\varepsilon^6, \qquad (19)$$

lying between the attainable bound (11) of $1+15\varepsilon^2+15\varepsilon^4+\varepsilon^6$ and the upper bound (9) of $1 + 15\varepsilon^2 + 75\varepsilon^4 + 125\varepsilon^6$. The matrix in (19) can be written in block form $\left(\begin{smallmatrix} C & D \\ -D & C \end{smallmatrix}\right)$, where C and D are 3×3 matrices.

When $\varepsilon \in (\varepsilon_1, 1]$, a larger determinant is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon & \varepsilon & \varepsilon & \varepsilon \\ \varepsilon & 1 & -\varepsilon & -\varepsilon & -\varepsilon & -\varepsilon \\ -\varepsilon & \varepsilon & 1 & \varepsilon & -\varepsilon & -\varepsilon \\ \varepsilon & -\varepsilon & -\varepsilon & 1 & -\varepsilon & -\varepsilon \\ -\varepsilon & \varepsilon & -\varepsilon & \varepsilon & 1 & -\varepsilon \\ -\varepsilon & \varepsilon & -\varepsilon & \varepsilon & -\varepsilon & 1 \end{vmatrix} = 1+3\varepsilon^2+32\varepsilon^3+63\varepsilon^4+48\varepsilon^5+13\varepsilon^6. \quad (20)$$

By equating the polynomials (19) and (20) we see that the crossover point $\varepsilon_1 \approx 0.3437$ is the real zero of the cubic $17\varepsilon^3 + 5\varepsilon^2 + 5\varepsilon - 3$.

When $\varepsilon \in (1, \infty)$, a larger determinant is

$$\begin{vmatrix} 1 & \varepsilon & \varepsilon & \varepsilon & \varepsilon & \varepsilon \\ \varepsilon & 1 & \varepsilon & \varepsilon & -\varepsilon & -\varepsilon \\ \varepsilon & \varepsilon & 1 & -\varepsilon & \varepsilon & -\varepsilon \\ -\varepsilon & -\varepsilon & \varepsilon & 1 & \varepsilon & -\varepsilon \\ -\varepsilon & \varepsilon & -\varepsilon & \varepsilon & 1 & -\varepsilon \\ -\varepsilon & \varepsilon & \varepsilon & -\varepsilon & -\varepsilon & 1 \end{vmatrix} = 1 + 3\varepsilon^2 + 16\varepsilon^3 + 15\varepsilon^4 + 125\varepsilon^6. \qquad (21)$$

The coefficient 125 of ε^6 in (21) is the maximal determinant of a 6×6 matrix with zero diagonal and elements in $[-1, 1]$. Similarly for the high-order coefficients in the other cases (12), (13), (14), and (18) that apply for large ε.

When $\varepsilon = 1$, all three of (19)–(21) give the maximal determinant 160 for 6×6 $\{\pm 1\}$-matrices [26, 39].

4.2 A condition for sharpness of Theorem 3

Theorem 4 gives a necessary and sufficient condition for the upper bound (9) of Theorem 3 to be best possible. An analogous result holds for the upper bound (8), by the transformation $\varepsilon \mapsto \varepsilon/(1+\varepsilon)$.

Theorem 4. *Let $H \in \mathbb{R}^{n\times n}$ be such that $|h_{ij}| \le 1$ for $1 \le i,j \le n$ and*

$$\det[(1-\varepsilon)I + \varepsilon H] = (1+(n-1)\varepsilon^2)^{n/2} \tag{22}$$

for all $\varepsilon \in (0, \varepsilon_0)$, where ε_0 is some positive constant. Then H is a skew-Hadamard matrix. Conversely, if H is a skew-Hadamard matrix of order n, then equation (22) holds for all $\varepsilon \in \mathbb{R}$.

Proof. First suppose that (22) holds for all $\varepsilon \in (0, \varepsilon_0)$. The left-hand side of (22) is a polynomial of degree n in ε, say $P(\varepsilon)$. The right-hand side of (22), say $Q(\varepsilon)$, is a polynomial if and only if $n = 1$ or $2|n$. If $Q(\varepsilon)$ is a polynomial, then it must be identically equal to $P(\varepsilon)$, since the two polynomials agree on a non-empty open set. Thus, (22) must hold for all $\varepsilon > 0$, in particular for $\varepsilon = 1$. Substituting $P(1) = Q(1)$ shows that $\det(H) = n^{n/2}$. Since $|h_{ij}| \le 1$, it follows that H is a Hadamard matrix.

Expanding $\det[(1-\varepsilon)I + \varepsilon H]$ in ascending powers of ε, we see that

$$\det[(1-\varepsilon)I + \varepsilon H] = \prod_{i=1}^{n}(1+(h_{ii}-1)\varepsilon) + O(\varepsilon^2) = 1 + \varepsilon\sum_{i=1}^{n}(h_{ii}-1) + O(\varepsilon^2).$$

Since the right-hand side of (22) is $1 + O(\varepsilon^2)$, we must have

$$\sum_{i=1}^{n}(h_{ii}-1) = 0,$$

but $h_{ii} \le 1$, so $h_{ii} = 1$ for $1 \le i \le n$. This proves that $\operatorname{diag}(H) = I$. Hence $\operatorname{diag}((1-\varepsilon)I + \varepsilon H) = I$.

Expanding $\det[(1-\varepsilon)I + \varepsilon H]$ again, and using $\operatorname{diag}[(1-\varepsilon)I + \varepsilon H] = I$, we see that

$$\det[(1-\varepsilon)I + \varepsilon H] = 1 - k\varepsilon^2 + O(\varepsilon^3),$$

where

$$k = \sum_{1 \le i < j \le n} h_{ij}h_{ji}\,.$$

The right-hand side of (22) is

$$1+\frac{n(n-1)}{2}\,\varepsilon^2+O(\varepsilon^3),$$

so $k=-n(n-1)/2$. Each of the $n(n-1)/2$ terms $h_{ij}h_{ji}$ is ± 1, so they must all be -1. Thus $(h_{ij},h_{ji})=(+1,-1)$ or $(-1,+1)$, implying that $h_{ij}+h_{ji}=0$ for all $i\neq j$. This proves that H is skew-Hadamard.

For the converse, suppose that H is a skew-Hadamard matrix of order n, and let $A=A(\varepsilon)=(1-\varepsilon)I+\varepsilon H$. Then, using $H^TH=nI$, we have

$$\begin{aligned}A^TA &= [(1-\varepsilon)I+\varepsilon H^T]\,[(1-\varepsilon)I+\varepsilon H]\\ &= [(1-\varepsilon)^2+2\varepsilon(1-\varepsilon)+n\varepsilon^2]\,I\\ &= [1+(n-1)\varepsilon^2]\,I.\end{aligned}$$

Thus

$$\det[A(\varepsilon)]^2=\det[A(\varepsilon)^TA(\varepsilon)]=(1+(n-1)\varepsilon^2)^n$$

and

$$\det[A(\varepsilon)]=\pm(1+(n-1)\varepsilon^2)^{n/2}. \tag{23}$$

Now $\det[A(\varepsilon)]>0$ for all sufficiently small ε, so the positive sign must apply in (23) for such ε. Since $\det[A(\varepsilon)]$ is a continuous function of ε, it follows that the positive sign must apply in (23) for all $\varepsilon\in\mathbb{R}$. Thus (22) holds for all $\varepsilon\in\mathbb{R}$. □

Acknowledgements

We thank L. N. (Nick) Trefethen for his comments and assistance with the references. The first author was supported in part by Australian Research Council grant DP140101417.

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