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The trace norm of r-partite graphs and matrices

La norme de trace des graphes et des matrices r-partis

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ABSTRACT

The trace norm of graphs has been widely studied under the name *graph energy*. This note presents bounds on the maximum trace norm of an r-partite graph of order n. The lower bounds come from conference and Hadamard matrices.

RÉSUMÉ

La norme de trace de graphes a été beaucoup étudiée sous le nom d'*énergie de graphe*. Cette note présente des bornes à la norme de trace maximale d'un graphe r-parti d'ordre n. Les bornes inférieures proviennent des matrices de conférence et de Hadamard.

1. Introduction and main results

The *trace norm* $\|A\|_*$ of a matrix A is the sum of the singular values of A, also known as the *nuclear norm* or the *Schatten* 1-*norm of* A. The trace norm of the adjacency matrix of graphs has been much studied under the name *graph energy*, a concept introduced by Gutman in [4]; for an overview of this vast research see [5]. Thus, write $\|G\|_*$ for the trace norm of the adjacency matrix of a graph G, and note that $\|G\|_*$ is just the sum of the absolute values of the eigenvalues of G.

Koolen and Moulton [9] studied which graphs of order n have maximum trace norm; in particular, they proved that if G is a graph of order n, then

$$\|G\|_* \leq n^{3/2}/2 + n/2, \tag{1}$$

with equality if and only if G belongs to a certain family of strongly regular graphs; in [6], Haemers showed that these graphs arise from a class of Hadamard matrices. Furthermore, Koolen and Moulton [10] proved that if G is a bipartite graph of order n, then

$$\|G\|_* \leq n^{3/2}/\sqrt{8} + n/2, \tag{2}$$

with equality if and only if G is the incidence graph of a particular type of design.

Given the cases of equality in bounds (1) and (2), arguably, much of their thrill is in the fact that the bulk parameter "trace norm" is maximized on rare graphs of delicate structure.

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To make the next step in this direction, recall that a graph is called *r-partite* if its vertices can be partitioned into r edgeless sets. We shall study the following problem arising in the vein of (2):

Problem 1. If $r \geq 3$, what is the maximum trace norm of an r-partite graph of order n?

For complete r-partite graphs the question was answered in [11], but in general, Problem 1 is much more difficult than the question for bipartite graphs, for it has many variations, it requires novel constructions, and most of it is beyond the reach of present methods.

First, we shall restate Problem 1 in analytic matrix form and shall give some upper bounds. The matrix setup elucidates the main factors in the graph problem. Further, using graph-theoretic proofs, we shall fine-tune the upper bounds at the price of somewhat increased complexity.

We shall show that for infinitely many r our upper bounds are exact or tight up to low order terms. The intriguing point here is that the tightness of the bounds is known only if r is the order of a conference matrix, and since such matrices do not exist for all r, a lot of open problems arise.

1.1. Upper bounds

Given an $n \times n$ matrix $A = [a_{i,j}]$ and nonempty sets $I \subset [n]$ and $J \subset [n]$, write $A[I, J]$ for the submatrix of all $a_{i,j}$ with $i \in I$ and $j \in J$. An $n \times n$ matrix A is called *k-partite* if there is a partition of its index set $[n] = N_1 \cup \cdots \cup N_k$ such that $A[N_i, N_i] = 0$ for any $i \in [k]$.

Further, write A^* for the *Hermitian transpose* of A, and let $\|A\|_{\max} = \max_{i,j} |a_{i,j}|$. As usual, I_n and J_n stand for the identity and the all-ones matrices of order n; we let $K_n = J_n - I_n$.

Theorem 2. *Let $n \geq r \geq 2$, and let A be an $n \times n$ complex matrix with $\|A\|_{\max} \leq 1$. If A is r-partite, then*

$$\|A\|_* \leq n^{3/2}\sqrt{1 - 1/r}. \tag{3}$$

Equality holds if and only if all singular values of A are equal to $\sqrt{(1 - 1/r)\,n}$.

Proof. Let $A = [a_{i,j}]$, and let $\sigma_1, \ldots, \sigma_n$ be the singular values of A. Clearly,

$$\begin{aligned}\|A\|_*^2 &= (\sigma_1 + \cdots + \sigma_n)^2 \leq n\left(\sigma_1^2 + \cdots + \sigma_n^2\right) = n(\operatorname{tr}(AA^*)) \\ &= \sum_{i,j \in [n]} |a_{i,j}|^2 \leq n^2 - \sum_{i \in [r]} |N_i|^2 \leq n^2 - \frac{1}{r}n^2,\end{aligned}$$

completing the proof of (3). If equality holds in (3), then

$$(\sigma_1 + \cdots + \sigma_n)^2 = n\left(\sigma_1^2 + \cdots + \sigma_n^2\right) = (1 - 1/r)\,n^2,$$

and so $\sigma_1 = \cdots = \sigma_n = \sqrt{(1 - 1/r)\,n}$, completing the proof of Theorem 2. $\square$

Remark 1. A matrix $A = [a_{i,j}]$ that makes (3) an equality has a long list of further properties, e.g.: r divides n; the partition sets are of size n/r; if an entry $a_{i,j}$ is not in a diagonal block, then $|a_{i,j}| = 1$; and most importantly, $AA^* = (1 - 1/r)\,nI_n$. It seems hard to find for which r and n such matrices exist.

Next, from Theorem 2 we deduce a similar bound for nonnegative matrices, in particular, for graphs.

Theorem 3. *Let $n \geq r \geq 2$, and let A be an $n \times n$ nonnegative matrix with $\|A\|_{\max} \leq 1$. If A is r-partite, then*

$$\|A\|_* \leq \frac{n^{3/2}}{2}\sqrt{1 - 1/r} + (1 - 1/r)\,n.$$

Proof. For each $i \in [r]$, set $n_i = |N_i|$, and write K for the matrix obtained from J_n by zeroing $J[N_i, N_i]$ for all $i \in [r]$. Note that K is the adjacency matrix of the complete r-partite graph with vertex classes $N_1, \ldots, N_r$. Since K has no positive eigenvalue other than the largest one $\lambda_1(K)$, we see that $\|K\|_* = 2\lambda_1(K)$. A result of Cvetković [2] (see also [3]) implies that $\lambda_1(K) \leq (1 - 1/r)\,n$, and so $\|K\|_* \leq 2(1 - 1/r)\,n$.

Now, let $B := 2A - K$, and note that the matrix B and the sets $N_1, \ldots, N_r$ satisfy the premises of Theorem 2; hence, using the triangle inequality, we find that

$$n^{3/2}\sqrt{1-1/r} \geq \|B\|_* \geq \|2A-K\|_* \geq 2\|A\|_* - \|K\|_* \geq 2\|A\|_* - 2(1-1/r)n,$$

completing the proof of Theorem 3. □

Note that the matrix A in Theorems 2 and 3 needs not be symmetric; nonetheless, the following immediate corollary gives precisely Koolen and Moulton's bound (2) if $r = 2$.

Corollary 4. *Let $n \geq r \geq 2$. If G is an r-partite graph of order n, then*

$$\|G\|_* \leq \frac{n^{3/2}}{2}\sqrt{1-1/r} + (1-1/r)n. \tag{4}$$

For $r \geq 3$ bound (4) can be improved by more involved methods. To this effect, first we shall give an upper bound on the trace norm of an r-partite graph with n vertices and m edges. Hereafter, $\lambda_i(G)$ stands for the i'th largest eigenvalue of the adjacency matrix of a graph G.

Theorem 5. *Let $n > r > 2$ and $2m \geq r^2 n$. If G is an r-partite graph with n vertices and m edges, then*

$$\|G\|_* \leq \frac{4m}{n} + \sqrt{(n-r)\left(2m - \frac{r}{r-1}\left(\frac{2m}{n}\right)^2\right)}. \tag{5}$$

Equality holds if and only if the following three conditions are met:

(i) *G is a regular graph;*
(ii) *the $r-1$ smallest eigenvalues of G satisfy*

$$\lambda_n(G) = \cdots = \lambda_{n-r+2}(G) = -\frac{2m}{(r-1)n};$$

(iii) *the eigenvalues $\lambda_2(G), \ldots, \lambda_{n-r+1}(G)$ satisfy*

$$\lambda_2^2(G) = \cdots = \lambda_{n-r+1}^2(G) = \frac{1}{n-r}\left(2m - \frac{r}{r-1}\left(\frac{2m}{n}\right)^2\right).$$

Proof. Let the graph G satisfy the premises of the theorem, and for short, write λ_i for $\lambda_i(G)$. Using the fact that $\lambda_1^2 + \cdots + \lambda_n^2 = 2m$ and the AM-QM inequality, we see that

$$\begin{aligned}
\|G\|_* &= \lambda_1 + \sum_{i=2}^{n-r+1}|\lambda_i| + \sum_{i=n-r+2}^{n}|\lambda_i| \leq \lambda_1 + \sum_{i=n-r+2}^{n}|\lambda_i| + \sqrt{(n-r)\sum_{i=2}^{n-r+1}\lambda_i^2} \\
&= \lambda_1 + \sum_{i=n-r+2}^{n}|\lambda_i| + \sqrt{(n-r)\left(2m - \lambda_1^2 - \sum_{i=n-r+2}^{n}|\lambda_i|^2\right)} \\
&\leq \lambda_1 + \sum_{i=n-r+2}^{n}|\lambda_i| + \sqrt{(n-r)\left(2m - \lambda_1^2 - \frac{1}{r-1}\left(\sum_{i=n-r+2}^{n}|\lambda_i|\right)^2\right)}.
\end{aligned}$$

Since G is r-partite, Hoffman's bound [7] implies that

$$\lambda_1 \leq |\lambda_{n-r+2}| + \cdots + |\lambda_n|.$$

Now, letting $x = \lambda_1$, $y = |\lambda_{n-r+2}| + \cdots + |\lambda_n|$, and $2m = A$, we maximize the function

$$f(x,y) := x + y + \sqrt{(n-r)\left(A - x^2 - \frac{1}{r-1}y^2\right)},$$

subject to the constraints

$$n \geq r \geq 3, \quad A \geq r^2 n, \quad y \geq x \geq A/n, \quad x^2 + \frac{1}{r-1}y^2 \leq A.$$

Using calculus, one finds that $f(x, y) < f(A/n, A/n)$, unless $y = x = A/n$. This proves (5).

Suppose that equality holds in (5). Clause (i) follows from $\lambda_1 = 2m/n$. Clause (ii) follows from $\lambda_{n-r+2} + \cdots + \lambda_n = -\lambda_1$ and

$$\sum_{i=n-r+2}^{n} \lambda_i^2 = \frac{1}{r-1}\left(\sum_{i=n-r+2}^{n} |\lambda_i|\right)^2.$$

Clause (iii) follows from

$$\sum_{i=2}^{n-r+1} \lambda_i^2 = \frac{1}{n-r}\left(\sum_{i=2}^{n-r+1} |\lambda_i|\right)^2 \quad \text{and} \quad \sum_{i=2}^{n-r+1} \lambda_i^2 = 2m - \lambda_1^2 - \sum_{i=n-r+2}^{n} \lambda_i^2,$$

completing the proof of Theorem 5. □

Next, we maximize bound (5) over m and get a bound that depends only on r and n. We omit this calculation and state only the final result:

Theorem 6. *Let $r \geq 2$ and $n \geq 4(r-1)^2$. If G is an r-partite graph of order n, then*

$$\|G\|_* \leq \frac{n(n-r)}{2\sqrt{(n-r)\frac{r}{r-1}+4}} + \frac{(r-1)n}{r} + \frac{2(r-1)n}{r\sqrt{(n-r)\frac{r}{r-1}+4}}. \tag{6}$$

Equality holds if and only if the following three conditions are met:

(i) *G is a regular graph of degree*

$$\left(1 + \frac{2}{\sqrt{(n-r)\frac{r}{r-1}+4}}\right)\frac{(r-1)n}{2r};$$

(ii) *the $r-1$ smallest eigenvalues of G satisfy*

$$\lambda_n(G) = \cdots = \lambda_{n-r+2}(G) = -\left(1 + \frac{2}{\sqrt{(n-r)\frac{r}{r-1}+4}}\right)\frac{n}{2r}.$$

(iii) *the eigenvalues $\lambda_2(G), \ldots, \lambda_{n-r+1}(G)$ satisfy*

$$|\lambda_2(G)| = \cdots = |\lambda_{n-r+1}(G)| = \frac{n}{2\sqrt{(n-r)\frac{r}{r-1}+4}}.$$

Remark 2. It is possible that bound (6) is exact for infinitely many r and n. In general, it can be shown, that (6) is better than (4) as long as $n > 4(r-1)^2$, but the difference between their right sides never exceeds some constant that is independent of n.

1.2. Constructions

Recall that an *Hadamard matrix* of order n is an $n \times n$ matrix H with entries of modulus 1 and such that $HH^* = nI_n$; hence, all singular values of H are equal to $\sqrt{n}$. Also, a *conference matrix* of order n is an $n \times n$ matrix C with zero diagonal, with off-diagonal entries of modulus 1, and such that $CC^* = (n-1)I_n$; hence all singular values of C are equal to $\sqrt{n-1}$. For details on Hadamard and conference matrices the reader is referred to [1,8]. We shall write $\otimes$ for the Kronecker (tensor) multiplication of matrices.

First, we show that bound (3) in Theorem 2 is best possible for infinitely many n, whenever r is the order of a conference matrix.

Theorem 7. *Let r be the order of a conference matrix, and let k be the order of a Hadamard matrix. There exists an r-partite matrix A of order $n = rk$ with $\|A\|_{\max} = 1$ and such that $\|A\|_* = n^{3/2}\sqrt{1-1/r}$.*

Proof. Let C be a conference matrix of order r and H be a Hadamard matrix of order k. Let $A := C \otimes H$, and partition $[rk]$ into r consecutive segments $N_1, \ldots, N_r$ of length k; we see that $\|A\|_{\max} = 1$, and $A[N_i, N_i] = 0$ for any $i \in [r]$. Finally, we see that

$$\|A\|_* = \|C \otimes H\|_* = \|C\|_* \|H\|_* = r\sqrt{r-1}k^{3/2} = n^{3/2}\sqrt{1-1/r},$$

completing the proof of Theorem 7. □

Next, a modification of the above construction provides some matching lower bounds for Theorems 3 and 6, and Corollary 4.

Theorem 8. *Let r be the order of a real symmetric conference matrix. If k is the order of a real symmetric Hadamard matrix, then there is an r-partite graph G of order $n = rk$ with*

$$\|G\|_* \geq \frac{n^{3/2}}{2}\sqrt{1-1/r} - (1-1/r)\,n.$$

Proof. Let C be a real symmetric conference matrix of order r, and let H be a real symmetric Hadamard matrix of order k. Let $B := C \otimes H$, and partition $[rk]$ into r consecutive segments $N_1, \ldots, N_r$ of length k. We see that $B[N_i, N_i] = 0$ for any $i \in [r]$, and also $B[N_i, N_j]$ is a $(-1, 1)$-matrix whenever $i, j \in [r]$ and $i \neq j$. Finally, let

$$A := \frac{1}{2}\left(B + K_r \otimes J_k\right),$$

and note that A is a symmetric $(0, 1)$-matrix, and $A[N_i, N_i] = 0$ for any $i \in [r]$. Hence A is the adjacency matrix of an r-partite graph G of order n. Note that the singular values of B are equal to $\sqrt{k(r-1)} = \sqrt{(1-1/r)\,n}$. Thus, using the triangle inequality, we find that

$$\|(B + K_n \otimes J_k)\|_* \geq \|B\|_* - \|K_r \otimes J_k\|_* \geq n^{3/2}\sqrt{1-1/r} - 2\,(r-1)\,k,$$

and so,

$$\|G\|_* \geq \frac{n^{3/2}}{2}\sqrt{1-1/r} - (1-1/r)\,n,$$

completing the proof of Theorem 8. □

Remark 3. For explicit examples, recall Paley's constructions: if q is an odd prime power, there is a real conference matrix of order $q+1$, which is symmetric if $q = 1 \pmod 4$; there is a real Hadamard matrix of order $q+1$ if $q = 3 \pmod 4$; there is a real symmetric Hadamard matrix of order $2\,(q+1)$ if $q = 1 \pmod 4$.

Remark 4. An extended version of this note can be found in arXiv:1502.04342.

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