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Beyond graph energy: Norms of graphs and matrices



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ABSTRACT

In 1978 Gutman introduced the energy of a graph as the sum of the absolute values of graph eigenvalues, and ever since then graph energy has been intensively studied.

Since graph energy is the trace norm of the adjacency matrix, matrix norms provide a natural background for its study. Thus, this paper surveys research on matrix norms that aims to expand and advance the study of graph energy.

The focus is exclusively on the Ky Fan and the Schatten norms, both generalizing and enriching the trace norm. As it turns out, the study of extremal properties of these norms leads to numerous analytic problems with deep roots in combinatorics.

The survey brings to the fore the exceptional role of Hadamard matrices, conference matrices, and conference graphs in matrix norms. In addition, a vast new matrix class is studied, a relaxation of symmetric Hadamard matrices.

The survey presents solutions to just a fraction of a larger body of similar problems bonding analysis to combinatorics. Thus, open problems and questions are raised to outline topics for further investigation.

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1. Introduction

This paper overviews the current research on the Ky Fan and the Schatten matrix norms that aims to expand and push forward the study of graph energy.

Graph energy has been introduced by Gutman in 1978 [13] as the sum of the absolute values of the graph eigenvalues; since then its study has produced a monumental body of work, as witnessed by the references of the monograph [14]. One reckons that such an enduring interest must be caused by some truly special property of the graph energy parameter.

1.1. Graph energy as a matrix norm

To crack the mystery of graph energy, it may be helpful to view it as the trace norm of the adjacency matrix. Recall that the *trace norm* $\|A\|_*$ of a matrix A is the sum of its singular values, which for a real symmetric matrix are just the moduli of its eigenvalues.

Hence, if G is graph with adjacency matrix A, then the energy of G is the trace norm of A.

This simple observation, made in [31], triggered some sort of a chain reaction. On the one hand, usual tools for norms provided new techniques for graph energy; see, e.g., [2,9,10,42]. On the other hand, viewed as a trace norm, graph energy was extended to non-symmetric and even to non-square matrices, and gave rise to new topics like "skew energy" and "incidence energy", see, e.g., [1,15–17,45,46,48].

To follow this track further, we need a few definitions. Write $M_{m,n}$ for the space of the $m \times n$ complex matrices.

Definition 1.1. A matrix norm is a nonnegative function $\|\cdot\|$ defined on $M_{m,n}$ such that:

- (a) ||A|| = 0 if and only if A = 0;
- (b) ||cA|| = |c| ||A|| for every complex number c;
- (c) $||A + B|| \le ||A|| + ||B||$ for every $A, B \in M_{m,n}$.

Observe that the usual definition of matrix norm includes additional properties, but they are not used in this survey.

A simple example of a matrix norm is the max-norm $||A||_{\max}$ defined for any matrix $A := [a_{i,j}]$ as $||A||_{\max} := \max_{i,j} |a_{i,j}|$.

Another example of a matrix norm is the largest singular value of a matrix, also known as its *operator norm*.

By contrast, the spectral radius $\rho(A)$ of a square matrix A is not a matrix norm. Likewise, if $\lambda_1(A), \ldots, \lambda_n(A)$ are the eigenvalues of A, neither of the functions

$$g(A) := |\lambda_1(A)| + \dots + |\lambda_n(A)|$$
 and $h(A) := |\operatorname{Re} \lambda_1(A)| + \dots + |\operatorname{Re} \lambda_n(A)|$

is a matrix norm. Indeed, if A is an upper triangular matrix with zero diagonal, then $\rho(A) = g(A) = h(A) = 0$, violating condition (a). Worse yet, if A is the adjacency matrix

of a nonempty graph G, and if A_U and A_L are the upper and lower triangular parts of A, then $A = A_U + A_L$, whereas $\rho(A) > \rho(A_U) + \rho(A_L) = 0$, $g(A) > g(A_U) + g(A_L) = 0$, and $h(A) > h(A_U) + h(A_L) = 0$, violating the triangle inequality.

Notwithstanding the importance of $\rho(A)$, g(A) and h(A), we reckon that if a matrix parameter naturally extends graph energy, it must obey at least conditions (a)–(c).

Further, any matrix norm $\|\cdot\|$ defined on $M_{n,n}$ can be extended to graphs of order n by setting $\|G\| := \|A\|$, where A is the adjacency matrix of G. Thus, we write $\|G\|_*$ for the energy of a graph G.

In this survey we deal exclusively with the Ky Fan and the Schatten norms, both defined via singular values. Recall that the *singular values* of a matrix A are the square roots of the eigenvalues of A^*A , where A^* is the conjugate transpose of A. We write $\sigma_1(A), \sigma_2(A), \ldots$ for the singular values of A arranged in descending order.

We write I_n for the identity matrix of order n, and $J_{m,n}$ for the $m \times n$ matrix of all ones; we let $J_n = J_{n,n}$. The Kronecker product of matrices is denoted by \otimes . Recall that the singular values of $A \otimes B$ are the products of the singular values of A and the singular values of B, with multiplicities counted.

Finally, we call a matrix regular, if its row sums are equal, and so are its column sums. Note that the adjacency matrix of a regular graph is regular, and the biadjacency matrix of a bipartite semiregular graph is also regular; these facts explains our choice for the term "regular". It is not hard to show that a matrix $A \in M_{m,n}$ is regular if and only if A has a singular value with singular vectors that are collinear to the all-ones vectors $\mathbf{j}_n \in \mathbb{R}^n$ and $\mathbf{j}_m \in \mathbb{R}^m$.

Weyl's inequality for singular values

For reader's sake we state Weyl's inequality for the singular values of sums of matrices (see, e.g., [20], p. 454), which we shall use on several occasions:

Let $n \ge m \ge 1$, $A \in M_{m,n}$ and $B \in M_{m,n}$. If $i \ge 1$, $j \ge 1$, and $i + j \le m + 1$, then

$$\sigma_{i+j-1}(A+B) \le \sigma_i(A) + \sigma_j(B). \tag{1}$$

The Power Mean inequality

For convenience, we also state the Power Mean (=PM) inequality:

If q > p > 0, and x_1, \ldots, x_n are nonnegative real numbers, then

$$\left(\frac{x_1^p + \dots + x_n^p}{n}\right)^{1/p} \le \left(\frac{x_1^q + \dots + x_n^q}{n}\right)^{1/q},$$

with equality holding if and only if $x_1 = \cdots = x_n$.

If p = 1 and q = 2, the PM inequality is called the Arithmetic Mean–Quadratic Mean (=AM-QM) inequality.

1.2. The Koolen and Moulton bound via norms

To illustrate the extreme fitness of matrix norms for the study of graph energy, we shall use norms to derive and extend the well-known result of Koolen and Moulton [23]:

If G is a graph of order n, then

$$||G||_* \le \frac{n\sqrt{n}}{2} + \frac{n}{2},$$
 (2)

with equality holding if and only if G belongs to a specific family of strongly regular graphs.

We shall show that in fact inequality (2) has nothing to do with graphs. Indeed, suppose that A is an $n \times n$ nonnegative matrix with $||A||_{\max} \leq 1$, and let $H := 2A - J_n$. Obviously, $||H||_{\max} \leq 1$, and the AM-QM inequality implies that

$$||H||_{*} = \sigma_{1}(H) + \dots + \sigma_{n}(H) \leq \sqrt{n\left(\sigma_{1}^{2}(H) + \dots + \sigma_{n}^{2}(H)\right)}$$
(3)

$$= \sqrt{n \operatorname{tr}(HH^*)} = \|H\|_2 \sqrt{n} \le n\sqrt{n}. \tag{4}$$

Now, the triangle inequality for the trace norm yields

$$||2A||_* = ||H + J_n||_* \le ||H||_* + ||J_n||_* \le n\sqrt{n} + n,$$

and so,

$$||A||_* \le \frac{n\sqrt{n}}{2} + \frac{n}{2}.\tag{5}$$

Therefore, if A is the adjacency matrix of a graph G, then (2) follows. That's it. Now, we give a necessary and sufficient condition for equality in (5):

Proposition 1.2. If A is an $n \times n$ nonnegative matrix with $||A||_{\max} \leq 1$, then equality holds in (5) if and only if the matrix $H := 2A - J_n$ is a regular Hadamard matrix.

Proof. If A forces equality in (5), then equalities hold throughout (3) and (4); hence, H is a (-1,1)-matrix and all singular values of H are equal to \sqrt{n} . Therefore, H is an Hadamard matrix (see Proposition 2.1 for details).

To show that H is regular, note that for every $i=2,\ldots,n$, Weyl's inequality (1) implies that

$$\sigma_i(2A) \le \sigma_{i-1}(H) + \sigma_2(J_n) = \sqrt{n}.$$

Since equality holds in (5), we find that

$$\sigma_1(2A) \ge n\sqrt{n} + n - (n-1)\sqrt{n} = \sqrt{n} + n = \sigma_1(H) + \sigma_1(J_n).$$

On the other hand, letting $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^n$ be unit singular vectors to $\sigma_1(2A)$, we see that

$$\sigma_1(2A) = \langle 2A\mathbf{x}, \mathbf{y} \rangle = \langle H\mathbf{x}, \mathbf{y} \rangle + \langle J_n \mathbf{x}, \mathbf{y} \rangle \le \sigma_1(H) + \sigma_1(J_n). \tag{6}$$

The latter inequality holds, for if B is an $m \times n$ real matrix, then

$$\sigma_1(B) = \max \left\{ \langle B\mathbf{x}, \mathbf{y} \rangle : \mathbf{x} \in \mathbb{R}^n, \ \mathbf{y} \in \mathbb{R}^m, \ \|\mathbf{x}\|_2 = \|\mathbf{y}\|_2 = 1 \right\}.$$

Therefore, equality holds in (6), and so \mathbf{x} and \mathbf{y} are singular vectors to $\sigma_1(H)$ and to $\sigma_1(J_n)$ as well; hence, $\mathbf{x} = \mathbf{y} = n^{-1/2}\mathbf{j}_n$, and so H is regular. This completes the proof of the "only if" part of Proposition 1.2; we omit the easy "if" part. \square

For graphs, Proposition 1.2 has to be modified accordingly:

Corollary 1.3. If G is a graph of order n with adjacency matrix A, then G forces equality in (2) if and only if the matrix $H := 2A - J_n$ is a regular symmetric Hadamard matrix, with -1 along the main diagonal.

Undeniably, the above arguments shed additional light on the inequality of Koolen and Moulton (2). Indeed, we realize that it is not about graphs—it is an analytic result about nonnegative matrices with bounded entries, with no symmetry or zero diagonal required. We also see that the triangle inequality is extremely efficient in graph energy problems, and can save pages of calculations.

Finally and most importantly, Proposition 1.2 (noted for graphs by Haemers in [18]) gives a sharper description of the extremal graphs and matrices, and exhibits the strong bonds between matrix norms and Hadamard matrices. It should be noted that similar ideas have been outlined by Božin and Mateljević in [5], but their study remained restricted to symmetric matrices.

1.3. The Ky Fan and the Schatten norms

The trace norm is the intersection of two fundamental infinite classes of matrix norms, namely the Schatten p-norms and the Ky Fan k-norms, defined as follows:

Definition 1.4. Let $p \ge 1$ be a real number and let $n \ge m \ge 1$. If $A \in M_{m,n}$, the **Schatten** p-norm $||A||_p$ of A is given by

$$||A||_{n} := (\sigma_{1}^{p}(A) + \cdots + \sigma_{m}^{p}(A))^{1/p}.$$

Definition 1.5. Let $n \geq m \geq k \geq 1$. If $A \in M_{m,n}$, the **Ky Fan** k-norm $||A||_{[k]}$ is given by

$$||A||_{[k]} := \sigma_1(A) + \cdots + \sigma_k(A).$$

As already mentioned, if $A \in M_{m,n}$, then

$$||A||_* = ||A||_{[m]} = ||A||_1$$
.

Another important case is the Schatten 2-norm $\|A\|_2$, also known as the *Frobenius norm* or A. The norm $\|A\|_2$ satisfies the following equality, which can be checked directly

$$||A||_{2} = \sqrt{\sigma_{1}^{2}(A) + \dots + \sigma_{m}^{2}(A)} = \sqrt{\operatorname{tr}(AA^{*})} = \sqrt{\operatorname{tr}(A^{*}A)} = \sqrt{\sum_{i,j} |a_{ij}|^{2}}.$$
 (7)

Note that equality (7) is widely used in spectral graph theory, for if a graph G has m edges, then $||G||_2 = \sqrt{2m}$.

Since both the Schatten and the Ky Fan norms generalize graph energy, in [33,34,37], the author proposed to study these norms for their own sake. Recently some progress was reported in [36] and [38].

In fact, certain Schatten norms of graphs have already been studied in graph theory, albeit implicitly: if A is the adjacency matrix of a graph G, then $||G||_2^2 = \operatorname{tr} A^2 = 2e(G)$, and if $k \geq 2$, then $||G||_{2k}^{2k} = \operatorname{tr} A^{2k}$, and so $||G||_{2k}^{2k}/4k$ is the number of closed walks of length 2k in G.

This survey shows that research on the Schatten and the Ky Fan norms adds significant volume and depth to graph energy. Older topics are seen in new light and from new viewpoints, but most importantly, this research leads to deep and hard problems, whose solutions would propel the theory of graph energy to a higher level.

1.4. Extremal problems for norms

Arguably the most attractive problems in spectral graph theory are the extremal ones, with general form like:

If G is a graph of order n, with some property \mathcal{P} , how large or small can a certain spectral parameter S be?

Such extremal questions are crucial to spectral graph theory, for they are a sure way to connect the spectrum of a graph to its structure. Not surprisingly, extremal problems are the hallmark of the study on graph energy as well, with S being the trace norm and \mathcal{P} chosen from a huge variety of graph families.

Thus, our survey keeps expanding and promoting this emphasis, with property \mathcal{P} chosen among the basic ones, like: "all graphs", "bipartite", "r-partite", and " K_r -free", whereas the spectral parameter S is a Schatten or a Ky Fan norm. Hence, upper and lower bounds on these norms will be a central topic in our presentation.

Let us mention a striking tendency here: frequently global parameters like norms are maximized on rare matrices of delicate structure, as it happens, e.g., in (5). Naturally the possibility of finding such extremal structures adds a lot of thrill and appeal to these problems, for they throw bridges between distant corners of analysis and combinatorics.

We shall also discuss Nordhaus–Gaddum problems; to this end, let \overline{G} denote the complement of a graph G. A Nordhaus–Gaddum problem is of the following type:

Given a graph parameter p(G), determine

$$\max \left\{ p\left(G\right) + p(\overline{G}) : v\left(G\right) = n \right\}.$$

Nordhaus—Gaddum problems were introduced in [39], and subsequently studied for numerous graph parameters; see [3] for a comprehensive survey. In [38], Nordhaus—Gaddum problems were studied for matrices, with p(A) being a Ky Fan norm. As it turns out, these Nordhaus—Gaddum parameters are maximized on the adjacency matrices of conference graphs, also of delicate and rare structure.

1.5. Matrices vs. graphs

Somewhat surprisingly, results about energy of graphs often extend effortlessly to more general matrices, say, to nonnegative or even to complex rectangular ones. Such extensions usually shed extra light, sometimes on the original graph results, and sometimes on well-known matrix topics.

We saw such an extension in the case of inequality (2), and here is another one. Recall that in [34] the McClelland upper bound [27] was extended to rectangular matrices as:

Proposition 1.6. If $n \ge m \ge 2$ and $A \in M_{m,n}$, then

$$||A||_* \le \sqrt{m \, ||A||_2}.$$
 (8)

If in addition $||A||_{\max} \leq 1$, then

$$||A||_* \le m\sqrt{n} \tag{9}$$

Inequality (8) follows immediately by the AM–QM inequality, but the important point here is which matrices force equality in (8), and which in (9). As seen in Theorem 4.9 below, a matrix A forces equality in (8) if and only if $AA^* = aI_m$ for some a > 0. Hence, A forces equality in (9) if and only if A is a partial Hadamard matrix.

In short, among the complex $m \times n$ matrices with entries of modulus 1, partial Hadamard matrices are precisely those with trace norm equal to $m\sqrt{n}$. In particular, if n=m, these are the matrices with determinant equal to $n^{n/2}$; however, the latter characterization is unwieldy and of limited use, for if $n \neq m$, determinants are nonexistent, whereas the trace norm always fits the bill.

We shall give inequalities similar to (9) for various other norms. Usually their simple proofs proceed by the PM inequality, but a constructive description of the matrices that force equality may be quite hard, sometimes even hopeless. Nevertheless, we always discuss the cases of equality, for they are the most instructive bit.

1.6. Structure of the survey

The survey covers results of the papers [11,22,33,34,36–38], with proofs of the known results suppressed; however, results appearing here for the first time are proved in full.

Section 2 is dedicated to the trace norm, with heavy emphasis on matrices. It starts with an introduction of Hadamard and conference matrices, and continues with the maximum trace norm of r-partite graphs and matrices, followed by Nordhaus–Gaddum problems about the trace norm. The section closes with a collection of open problems about graphs with maximal energy.

Section 3 is about the Ky Fan norms, with emphasis on the maximal Ky Fan norms of graphs. In this topic, a crucial role plays a class of matrices extending real symmetric Hadamard matrices. We analyze this class and find the maximal Ky Fan k-norm of graphs for infinitely many k. We also survey Nordhaus–Gaddum problems and show a few relations of the clique and the chromatic numbers to Ky Fan norms.

Section 4 is dedicated to the Schatten norms. The section starts with a few results on the Schatten p-norm as a function of p. This direction is totally new, with no roots in the study of graph energy. The other topics of Section 4 are: graphs and matrices with extremal Schatten norms; r-partite matrices and graphs with maximal Schatten norms; Schatten norms of trees; and Schatten norms of random graphs.

2. The trace norm

We begin this section with a discussion of Hadamard and conference matrices, which are essential for bounds on the norms of graphs and matrices. In particular, we stress on several analytic characterizations of these matrices via their singular values, which are used throughout the survey.

In Section 2.2, we give bounds on the trace norms of rectangular complex and nonnegative matrices conceived in the spirit of graph energy. Particularly curious is Proposition 2.7—a "bound generator" that can be used to convert lower bounds on the operator norm into upper bounds on the trace norm.

In Section 2.3, we present results on the maximal trace norm of r-partite graphs and matrices, which recently appeared in [35]. This section brings conference matrices to the limelight; note that hitherto these matrices have been barely used in graph energy.

In Section 2.4, we outline solutions of some Nordhaus–Gaddum problems about the trace norm of nonnegative matrices and describe a tight solution to a problem of Gutman and Zhou. The section shows the exclusive role of the conference graphs for Nordhaus–Gaddum problems about the trace norm.

Finally, in Section 2.5, we raise a number of open problems about graphs of maximal energy, which suggest that in many directions we are yet to face the real difficulties in the study of graph energy.

2.1. Hadamard and conference matrices

Recall three well-known definitions:

An Hadamard matrix of order n is an $n \times n$ matrix H, with entries of modulus 1, such that $HH^* = nI_n$.

More generally, if $n \geq m$, a partial Hadamard matrix is an $m \times n$ matrix H, with entries of modulus 1, such that $HH^* = nI_m$.

A conference matrix of order n is an $n \times n$ matrix C with zero diagonal, with off-diagonal entries of modulus 1, such that $CC^* = (n-1)I_n$.

Unfortunately, the above definitions, albeit concise and sleek, fail to emphasize the crucial role of the singular values of these matrices. To make our point clear, we shall outline several characterizations via singular values. Obviously, all singular values of an $n \times n$ Hadamard matrix are equal to \sqrt{n} ; also, assuming that $m \le n$, all nonzero singular values of an $m \times n$ partial Hadamard matrix are equal to \sqrt{n} . Likewise, all singular values of an $n \times n$ conference matrix are equal to $\sqrt{n-1}$.

Proposition 2.1. If $H := [h_{i,j}]$ is an $n \times n$ complex matrix, with $|h_{i,j}| = 1$ for all $i, j \in [n]$, then the following conditions are equivalent:

- (i) H satisfies the equation $HH^* = nI_n$;
- (ii) each singular value of H is equal to \sqrt{n} ;
- (iii) $||H||_* = n\sqrt{n}$;
- (iv) the largest singular value of H is equal to \sqrt{n} ;
- (v) the smallest singular value of H is equal to \sqrt{n} .

Proof. The implications (i) \Rightarrow (ii) \Rightarrow (iii), (ii) \Rightarrow (iv), and (ii) \Rightarrow (v) are obvious. As in (3), we see that $||H||_* \leq n\sqrt{n}$, with equality if and only if $\sigma_1(H) = \cdots = \sigma_k(H) = \sqrt{n}$. Hence, (iii) \Rightarrow (ii).

To prove the implications (iv) \Rightarrow (i) and (v) \Rightarrow (i), note that the diagonal elements of HH^* are equal to n, as these are the inner product of the rows of H with themselves. Hence, if HH^* contains a nonzero off-diagonal element a, then HH^* contains a principal 2×2 matrix

$$B = \begin{bmatrix} n & \overline{a} \\ a & n \end{bmatrix}.$$

Clearly, the characteristic polynomial of B is $x^2 - nx + n^2 - |a|^2$, and so

$$\lambda_1(B) = n + |a|$$
 and $\lambda_2(B) = n - |a|$.

Now, Cauchy's interlacing theorem implies that

$$\sigma_1^2(H) = \lambda_1(HH^*) \ge \lambda_1(B) > \lambda_2(B) \ge \lambda_n(HH^*) = \sigma_n^2(H)$$
.

Therefore, if (i) fails, then both (iv) and (v) fail. Hence, the implications (iv) \Rightarrow (i) and (v) \Rightarrow (i) hold as well, completing the proof of Proposition 2.1. \Box

Proposition 2.1 immediately implies the following essential bound on the trace norm of complex square matrices.

Proposition 2.2. If A is an $n \times n$ matrix with $||A||_{\max} \leq 1$, then

$$||A||_* \le n\sqrt{n}$$
.

Equality holds if and only if all singular values of A are equal to \sqrt{n} . Equivalently, equality holds if and only if A is a Hadamard matrix.

The analytic characterizations (ii)–(v) in Proposition 2.1 are by far simpler and clearer than (i); in addition, we see that Hadamard matrices may be introduced and studied regardless of determinants, which obscure the picture in this case. This point of view is further supported by the seamless extension of Propositions 2.1 and 2.2 to nonsquare partial Hadamard matrices, where determinants simply do not exists. Here are the corresponding statements:

Proposition 2.3. Let $n \ge m \ge 2$. If $H := [h_{i,j}]$ is an $m \times n$ complex matrix, with $|h_{i,j}| = 1$ for all $i \in [m]$, $j \in [n]$, then the following conditions are equivalent:

- (i) H satisfies the equation $HH^* = nI_m$;
- (ii) each of the first m singular values of H is equal to \sqrt{n} ;
- (iii) $||H||_* = m\sqrt{n}$;
- (iv) the largest singular value of H is equal to \sqrt{n} ;
- (v) the smallest nonzero singular value of H is equal to \sqrt{n} .

Proposition 2.4. Let $n \ge m \ge 2$. If A is an $m \times n$ matrix with $||A||_{\max} \le 1$, then

$$||A||_* \le m\sqrt{n}.$$

Equality holds if and only if all nonzero singular values of A are equal to \sqrt{n} . Equivalently, equality holds if and only if A is a partial Hadamard matrix.

Finally, Propositions 2.1 and 2.2 can be adapted for conference matrices:

Proposition 2.5. If C is an $n \times n$ complex matrix with zero diagonal, with off-diagonal entries of modulus 1, then the following conditions are equivalent:

- (i) C satisfies the equation $CC^* = (n-1)I_n$;
- (ii) each singular value of C is equal to $\sqrt{n-1}$;
- (iii) $||C||_* = n\sqrt{n-1};$
- (iv) the largest singular value of C is equal to $\sqrt{n-1}$;
- (v) the smallest singular value of C is equal to $\sqrt{n-1}$.

Proposition 2.6. If A is an $n \times n$ matrix with zero diagonal and $||A||_{\max} \leq 1$, then

$$||A||_* \le n\sqrt{n-1}.$$

Equality holds if and only if all singular values of A are equal to $\sqrt{n-1}$. Equivalently, equality holds if and only if A is a conference matrix.

In summary: Hadamard, partial Hadamard, and conference matrices are unique solutions of basic extremal analytic problems about the trace norm. Moreover, the definitions of these matrices via singular values are simpler and clearer than the standard definitions.

2.2. The trace norm of general matrices

In this section we give several bounds on the trace norm of general matrices, which were proved in [31]. Most proofs are omitted here, but in Section 4.1 these results will be extended to Schatten norms and their proofs will be outlined.

We start with a strengthening of bound (8).

Proposition 2.7. If $n \geq m \geq 2$ and $A \in M_{m,n}$, then

$$||A||_{*} \le \sigma_{1}(A) + \sqrt{(m-1)(||A||_{2}^{2} - \sigma_{1}^{2}(A))}.$$
 (10)

Equality holds in (10) if and only if $\sigma_2(A) = \cdots = \sigma_m(A)$.

Inequality (10) merits closer attention. First, together with the Cauchy–Schwarz inequality, (10) implies the simple and straightforward inequality (8). What's more, in exchange for its clumsy form, inequality (10) provides extended versatility. Indeed, note that the function

$$f(x) := x + (m-1)^{-1/2} (||A||_2^2 - x^2)^{1/2}$$

is decreasing whenever $\|A\|_2/\sqrt{m} \le x \le \|A\|_2$. Since

$$||A||_{2}/\sqrt{m} \leq \sigma_{1}(A) \leq ||A||_{2},$$

if a number C satisfies

$$\sigma_1(A) \ge C \ge ||A||_2 / \sqrt{m}$$

then $f(\sigma_1(A)) \leq f(C)$, and so

$$||A||_* \le C + \sqrt{(m-1)\left(||A||_2^2 - C^2\right)}.$$

Therefore, Proposition 2.7 is a vehicle for converting lower bounds on $\sigma_1(A)$ into upper bounds on $||A||_*$. Lower bounds on $\sigma_1(A)$ have been studied, see, e.g., [30] for an infinite family of such bounds, which, under some restrictions may give an infinite family of upper bounds on $||A||_*$. In particular, note the following basic lower bounds on $\sigma_1(A)$:

Proposition 2.8. Let $A \in M_{m,n}$, let r_1, \ldots, r_m be the row sums of A, and let c_1, \ldots, c_n be its column sums. Then

$$\sigma_1(A) \ge \sqrt{\frac{1}{n} \left(|r_1|^2 + \dots + |r_m|^2 \right)},$$

 $\sigma_1(A) \ge \sqrt{\frac{1}{m} \left(|c_1|^2 + \dots + |c_n|^2 \right)},$

and

$$\sigma_1(A) \ge \frac{1}{\sqrt{mn}} \sum_{i} |r_i|. \tag{11}$$

If equality holds in (11), then $|r_1| = \cdots = |r_m|$. If A is nonnegative, equality holds in (11) if and only if A is regular.

Propositions 2.8 leads to three bounds on $||A||_*$; we spell out just one of them, generalizing a well-known result of Koolen and Moulton [23].

Proposition 2.9. Let $n \geq m \geq 2$ and $A = [a_{i,j}] \in M_{m,n}$. If

$$\frac{1}{\sqrt{mn}} \sum\nolimits_{i} \left| \sum\nolimits_{j} a_{ij} \right| \geq \sqrt{n} \left\| A \right\|_{2},$$

then

$$||A||_{*} \le \frac{1}{\sqrt{mn}} \sum_{i} \left| \sum_{j} a_{ij} \right| + \sqrt{(m-1) \left(||A||_{2}^{2} - \frac{1}{mn} \left(\sum_{i} \left| \sum_{j} a_{ij} \right| \right)^{2} \right)}.$$
 (12)

If equality holds in (12), then $\sigma_2(A) = \cdots = \sigma_m(A)$, the row sums of A are equal in absolute value and $\sigma_1(A) = (mn)^{-1/2} \sum_i \left| \sum_j a_{ij} \right|$.

If A is nonnegative, then equality holds in (12) if and only if A is regular and $\sigma_2(A) = \cdots = \sigma_m(A)$.

The conditions for equality in (10) and (12) are stated here for the first time, but we omit their easy proofs.

Next, we recall an absolute bound on $||A||_{*}$:

Proposition 2.10. Let $n \geq m \geq 2$ and let A be an $m \times n$ nonnegative matrix. If $\|A\|_{\max} \leq 1$, then

$$||A||_* \le \frac{m\sqrt{n}}{2} + \frac{\sqrt{mn}}{2}.$$
 (13)

Equality holds if and only if the matrix $2A - J_{m,n}$ is a regular partial Hadamard matrix.

Obviously, Proposition 2.10 generalizes Koolen and Moulton's result (2); inequality (13) is proved in [31], but the characterization of the equality is new. In turn, Proposition 2.10 is generalized in Theorems 3.5 and 4.13 below.

Let us note that for (0,1)-matrices Kharaghani and Tayfeh-Rezaie [22] have characterized the conditions for equality in inequality (13), using a different wording:

Theorem 2.11 ([22]). Let $n \ge m \ge 2$. If A is an $m \times n$ (0,1)-matrix, then

$$\|A\|_* \leq \frac{m\sqrt{n}}{2} + \frac{\sqrt{mn}}{2}.$$

Equality holds if and only if A is the incidence matrix of a balanced incomplete block design with parameters

$$m, n, n(m + \sqrt{m})/2m, (m + \sqrt{m})/2, n(m + 2\sqrt{m})/4m.$$

Observe that Proposition 2.10 and Theorem 2.11 have direct consequences for bipartite graphs. Indeed, the adjacency matrix A of a bipartite graph G can be written as a block matrix

$$A = \begin{bmatrix} 0 & B^T \\ B & 0 \end{bmatrix},$$

for some (0,1)-matrix B, which is called the biadjacency matrix of G.

Since every (0,1)-matrix is the biadjacency matrix of a certain bipartite graph, in a sense, the study of bipartite graphs is equivalent to the study of rectangular (0,1)-matrices. In particular, it is known that the spectrum of G consists of the nonzero singular values of B, together with their negatives and possibly some zeros; thus, if $\|\cdot\|$ is a Ky Fan or a Schatten norm, then

$$||G|| = 2 ||B||$$
.

Hence, studying norms of bipartite graphs is tantamount to studying norms of arbitrary (0, 1)-matrices. For instance, Proposition 2.10 extends the following result of Koolen and Moulton about bipartite graphs [24]:

If G is a bipartite graph of order n, then

$$||G||_* \le \frac{n\sqrt{n}}{2\sqrt{2}} + \frac{n}{2},\tag{14}$$

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

Finally, let us mention one lower bound on the trace norm of general matrices. Note that for any matrix A, $\sigma_2(A) \neq 0$ if and only if the rank of A is at least 2. For matrices of rank at least 2, the following lower bound was given in [31].

Proposition 2.12. If the rank of a matrix $A = [a_{i,j}]$ is at least 2, then

$$||A||_{*} \ge \sigma_{1}(A) + \frac{1}{\sigma_{2}(A)} \left(\sum_{i,j} |a_{ij}|^{2} - \sigma_{1}^{2}(A) \right).$$
 (15)

Equality holds if and only if all nonzero eigenvalues of G other than λ have the same absolute value.

Bound (15) is quite efficient for graphs: for example, equality holds in (15) if A is the adjacency matrix of a design graph, or a complete graph, or a complete bipartite graph; however, there are also other graphs whose adjacency matrix forces equality in (15).

Problem 2.13. Give a constructive characterization of all graphs G such that the nonzero eigenvalues of G other than its largest eigenvalue have the same absolute value.

2.3. The trace norm of r-partite graphs and matrices

In the previous section we saw that the inequality (14) of Koolen and Moulton can be extended using the biadjacency matrix of a bipartite graph. Inequality (14) can also be extended in another direction, namely to r-partite graphs for $r \ge 3$.

Recall that a graph is called r-partite if its vertices can be partitioned into r edgeless sets. Clearly, inequality (14) leads to the following natural problem:

Problem 2.14. What is the maximum trace norm of an r-partite graph of order n?

For complete r-partite graphs the question was answered in [6], but in general, Problem 2.14 is much more difficult, as, for almost all r and n, it requires constructions that presently are beyond reach. Nonetheless, some tight approximate results were obtained

recently in the paper [35] and in its ArXiv version. Below, we give an outline of these results, with their proofs suppressed. In Section 4, we prove somewhat stronger results for the Schatten norms.

First, we generalize the notion of r-partite graph to complex square matrices. To this end, given an $n \times n$ matrix $A = [a_{i,j}]$ and nonempty sets $I \subset [n]$, $J \subset [n]$, write A[I,J] for the submatrix of all $a_{i,j}$ with $i \in I$ and $j \in J$. Now, r-partite matrices are defined as follows:

Definition 2.15. An $n \times n$ matrix A is called r-partite if there is a partition of its index set $[n] = N_1 \cup \cdots \cup N_r$ such that $A[N_i, N_i] = 0$ for any $i \in [r]$.

Clearly, the adjacency matrix of an r-partite graph is an r-partite matrix, but our definition extends to any square matrix.

We continue with an upper bound on the trace norm of r-partite matrices. For a proof see the more general Theorem 4.40.

Theorem 2.16. Let $n \ge r \ge 2$, and let A be an $n \times n$ matrix with $||A||_{\max} \le 1$. If A is r-partite, then

$$||A||_* \le n^{3/2} \sqrt{1 - 1/r}. \tag{16}$$

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

The most challenging point of Theorem 2.16 is the case of equality in (16). Any matrix $A = [a_{i,j}]$ that forces equality in (16) has a long list of special properties, e.g.:

- -r divides n;
- all its partition sets are of size n/r;
- if an entry $a_{i,j}$ is not in a diagonal block, then $|a_{i,j}| = 1$;
- $-AA^* = (1 1/r) nI_n.$

We see that the rows of A are orthogonal, and so are its columns. Despite these many necessary conditions, it seems hard to find for which r and n such matrices exist.

Problem 2.17. Give a constructive characterization of all r-partite $n \times n$ matrices A with $||A||_{\max} \leq 1$ such that

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

We cannot solve this difficult problem in general, but nevertheless, we can show that if r is the order of a conference matrix, then equality holds in (16) for infinitely many r-partite matrices.

Theorem 2.18. Let r be the order of a conference matrix, and let k be the order of an Hadamard matrix. There exists an r-partite matrix A of order n = rk with $||A||_{\max} = 1$ such that

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

For a proof of Theorem 2.18 see the more general Theorem 4.41.

Complex Hadamard matrices of order n exists for any n. This is not true for conference matrices and real Hadamard matrices, although numerous constructions of such matrices are known, e.g., Paley's constructions, which are as follows:

If q is an odd prime power, then:

- 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 $q=1 \pmod{4}$.

It is known that there is no conference matrix of order 3, so we have an intriguing problem:

Problem 2.19. Let f(n) be the maximal trace norm of a tripartite matrix of order n, with $||A||_{\max} \leq 1$. Find

$$\lim_{n\to\infty} f(n) n^{-3/2}.$$

The existence of the above limit was proved in the ArXiv version of [35].

Next, we give an approximate solution of Problem 2.14. We state a bound for non-negative matrices, which is valid also for graphs.

Theorem 2.20. Let $n \ge r \ge 2$, and let A be an $n \times n$ nonnegative matrix with $||A||_{\max} \le 1$. If A is r-partite, then

$$||A||_* \le \frac{n^{3/2}}{2} \sqrt{1 - 1/r} + (1 - 1/r) n.$$
 (17)

For a proof of Theorem 2.20 see the more general Theorem 4.45.

Note that the matrix A in Theorems 2.16 and 2.20 needs not be symmetric; nonetheless, the following immediate corollary implies precisely Koolen and Moulton's bound (14) for bipartite graphs (r = 2).

Corollary 2.21. Let $n \ge r \ge 2$. If G is an r-partite graph of order n, then

$$||G||_* \le \frac{n^{3/2}}{2} \sqrt{1 - 1/r} + (1 - 1/r) n.$$
 (18)

The linear in n term in the right sides of bounds (17) and (18) can be diminished for $r \geq 3$ by more involved methods; see the ArXiv version of [35]. However, the improved bounds in [35] are quite complicated and leave no hope for expressions as simple as in (14).

Further, the construction in Theorem 2.18 can be modified to provide matching lower bounds for Theorem 2.20 and Corollary 2.21. For a proof of Theorem 2.22 see Theorem 4.47.

Theorem 2.22. 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

$$||G||_* \ge \frac{n^{3/2}}{2} \sqrt{1 - 1/r} - (1 - 1/r) n.$$
 (19)

Note that bounds (18) and (19) differ only in their linear terms; however, getting rid of this difference seems very hard, and needs improvements in both (18) and (19).

2.4. Nordhaus-Gaddum problems for the trace norm

Let G be a graph G of order n. It seems not widely known that the energy of the complement \overline{G} of G is not too different from the energy of G. Indeed, if A and \overline{A} are the adjacency matrices of G and \overline{G} , then $A + \overline{A} = J_n - I_n$ and using the triangle inequality for the trace norm, we find that

$$\|\overline{A}\|_{*} = \|J_n - I_n - A\|_{*} \le \|A\|_{*} + \|J_n - I_n\|_{*} = \|G\|_{*} + 2n - 2.$$

By symmetry, we get the following proposition:

Proposition 2.23. If G is a graph of order n and \overline{G} is the complement of G, then

$$\left| \left\| \overline{G} \right\|_* - \left\| G \right\|_* \right| \le 2n - 4. \tag{20}$$

Equality in (20) holds if and only if G or \overline{G} is a complete graph.

Inequality (20) can be made more precise using Weyl's inequalities for the eigenvalues of Hermitian matrices:

Proposition 2.24. If G is a graph of order n and \overline{G} is the complement of G, then

$$\|G\|_* - \|\overline{G}\|_* \le 2\lambda_1(G)$$

and

$$\|\overline{G}\|_* - \|G\|_* \le 2\lambda_1(\overline{G}).$$

It seems that the bounds in Proposition 2.24 can be improved, so we raise the following problem:

Problem 2.25. Find the best possible upper bounds for $||G||_* - ||\overline{G}||_*$ for general and for regular graphs.

As shown by Koolen and Moulton in [23], G satisfies $||G||_* = n\sqrt{n}/2 + n/2$ if and only if G is a strongly regular graph with parameters

$$(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4).$$
 (21)

Hence, if $||G||_* = n\sqrt{n}/2 + n/2$, it is not hard to see that the complement \overline{G} satisfies $||\overline{G}||_* < n\sqrt{n}/2 + n/2$. This observation led Gutman and Zhou [47] to the following natural problem:

Problem 2.26. What is the maximum $\mathcal{E}(n)$ of the sum $\|G\|_* + \|\overline{G}\|_*$, where G is a graph of order n?

In [47], Gutman and Zhou proved a tight upper bound on $\mathcal{E}(n)$:

$$\mathcal{E}(n) \le (n-1)\sqrt{n-1} + \sqrt{2}n. \tag{22}$$

Clearly, Problem 2.26 is a Nordhaus–Gaddum problem for the trace norm of graphs. Before discussing Problem 2.26 further, we introduce conference and Paley graphs:

Definition 2.27. A **conference graph** of order n is a strongly regular graph with parameters

$$(n, (n-1)/2, (n-5)/4, (n-1)/4).$$

It is easy to see that the eigenvalues of a conference graph of order n are

$$(n-1)/2, ((\sqrt{n}-1)/2)^{[(n-1)/2]}, (-(\sqrt{n}+1)/2)^{[(n-1)/2]},$$

where the numbers in brackets denote multiplicities. Note that the complement of a conference graph is also a conference graph. The best known examples of conference graphs are the Paley graphs P_q , which are defined as follows:

Given a prime power $q = 1 \pmod{4}$, the vertices of P_q are the numbers $1, \ldots, q$ and two vertices u, v are adjacent if |u - v| is an exact square mod q.

Additional introductory and reference material on conference and Paley graphs can be found, e.g., in [12].

Returning to Problem 2.26, note that any conference graph of order n provides the lower bound

$$\mathcal{E}(n) \ge (n-1)\sqrt{n} + n - 1,\tag{23}$$

which matches the upper bound of Gutman and Zhou (22) up to a linear term.

In [38], it was shown that conference graphs are, in fact, extremal for Problem 2.26, as shown in the following more general matrix statement:

Theorem 2.28. Let $n \geq 7$, and let A be an $n \times n$ symmetric nonnegative matrix with zero diagonal. If $||A||_{\max} \leq 1$, then

$$||A||_{*} + ||J_{n} - I_{n} - A||_{*} \le (n-1)\sqrt{n} + n - 1, \tag{24}$$

with equality holding if and only if A is the adjacency matrix of a conference graph.

The proof of Theorem 2.28 is not easy and involves some new analytic and combinatorial techniques using Weyl's inequalities for sums of Hermitian matrices. It is based on the following two results of separate interest.

Theorem 2.29. Let A be an $n \times n$ nonnegative matrix with zero diagonal. If $||A||_{\max} \leq 1$, then

$$\left\| A + \frac{1}{2} I_n \right\|_* + \left\| J_n - A - \frac{1}{2} I_n \right\|_* \le (n-1)\sqrt{n} + n.$$
 (25)

Equality holds if and only if A is a (0,1)-matrix, with all row and column sums equal to (n-1)/2, and with $\sigma_i\left(A+\frac{1}{2}I_n\right)=\sqrt{n}/2$ for every $i=2,\ldots,n$.

Corollary 2.30. Let A be an $n \times n$ symmetric nonnegative matrix with zero diagonal and with $||A||_{\max} \leq 1$. If

$$\left\| A + \frac{1}{2} I_n \right\|_{*} + \left\| J_n - A - \frac{1}{2} I_n \right\|_{*} = (n-1)\sqrt{n} + n, \tag{26}$$

then A is the adjacency matrix of a conference graph.

Let us note that the difficulty of the proof of Theorem 2.28 stems from the stipulations that A is symmetric and its diagonal is zero. In Section 3, Theorem 3.21, we shall see that if these constraints are omitted, one can prove a sweeping generalization for any Ky Fan norm, but it is not tight for graphs. For convenience, here we state that result for the trace norm:

Theorem 2.31. If $n \ge m$ and A is an $m \times n$ nonnegative matrix with $||A||_{\max} \le 1$, then

$$||A||_* + ||J_{m,n} - A||_* \le \sqrt{m(m-1)n} + \sqrt{mn}.$$
 (27)

Equality holds in (27) if only if A is a (0,1)-matrix with

$$\sigma_1(A) = \sigma_1(\overline{A}) = \sqrt{mn}/2$$

and

$$\sigma_2(A) = \dots = \sigma_m(A) = \sigma_2(\overline{A}) = \dots = \sigma_m(\overline{A}) = \frac{1}{2}\sqrt{\frac{mn}{m-1}}.$$

Equivalently, equality holds in (27) if only if the matrix $H := 2A - J_{m,n}$ has zero row sums and column sums and

$$\sigma_1(H) = \dots = \sigma_{m-1}(H) = \sqrt{\frac{mn}{m-1}}.$$

2.5. Some open problems on graph energy

Bounds (2), (14), Proposition 2.9, Theorem 2.11 may leave the false impression that the problems about graphs of maximal energy are essentially solved. This is far from being true. Indeed, in all these cases we have concise upper bounds, together with descriptions of sparse sets of graphs for which these bounds are attained. Unfortunately these descriptions are non-constructive and hinge on the unclear existence of combinatorial objects like Hadamard matrices, strongly regular graphs, or BIBDs. What's more, even if we knew all about these special cases of equality, we still know nothing about the general case, which may considerably deviate from the special cases.

Obviously, in such problems we have to follow the customary path of extremal graph theory: that is to say, we have to define and investigate a particular extremal function. For instance, for the energy, we have to define the function

$$F_*(n) := \max \{ \|G\|_* : G \text{ is a graph of order } n \},$$

and come to grips with the following problem:

Problem 2.32. Find or approximate $F_*(n)$ for every n.

To solve this problem we must give upper and lower bounds on $F_*(n)$, aiming to narrow the gap between them as much as possible. Note that the closing of these bounds may go in rounds for decades.

Let us note that the lower bounds on $F_*(n)$ and on similar extremal functions are usually based on constructions. For example, a simple construction using the Paley graphs [32] shows that

$$F_*(n) \ge \frac{n\sqrt{n}}{2} - n^{11/10}.$$

Improving this bound significantly is a major problem, mostly because of its relation to possible orders of Hadamard matrices. Perhaps $F_*(n) \ge n^{3/2}/2$ for sufficiently large n, but this is far from clear.

Let us state a few more problems of similar type.

Problem 2.33. For every n, find or approximate the function

 $\max \{ \|G\|_* : G \text{ is a bipartite graph of order } n \}.$

In fact, Problem 2.33 can be extended to a two-parameter version, for which results on partial Hadamard matrices [25] may provide some solutions:

Problem 2.34. Let $q \geq p \geq 1$. Find or approximate the function

 $\max \{ \|G\|_* : G \text{ is a bipartite graph with vertex classes of sizes } p \text{ and } q \}.$

At that point, Problem 2.14 comes in mind, but we shall not restate it again. Instead, as it is unlikely that it will be solved satisfactorily in the nearest future, we state the following simplified version of it:

Problem 2.35. Let $f_r(n)$ be the maximal trace norm of an r-partite graph of order n. Find

$$\lim_{n\to\infty} f_r(n) n^{-3/2}.$$

Note that the existence of the above limit was proved in the ArXiv version of [35]. Next, in the spirit of the famous Turán theorem [44], we raise the following, probably difficult, problem:

Problem 2.36. Let $r \geq 2$. Find or approximate the function

 $g_{r}\left(n\right)=\max\left\{ \left\Vert G\right\Vert _{\ast}:G\text{ is a graph with no complete subgraph of order }r+1\right\} .$

The author knows nothing even for $g_2(n)$. Since finding precisely $g_r(n)$ for any $r \geq 2$ seems difficult, it is worth to consider the following simpler question:

Problem 2.37. Does the limit

$$\gamma_r = \lim_{n \to \infty} g_r(n) \, n^{-3/2}$$

exist? If yes, find γ_r .

Finally, we shall discuss two problems with a different setup. Let G be a graph of order n with m edges. In [23], Koolen and Moulton showed that if $m \ge n/2$, then

$$||G||_* \le 2m/n + \sqrt{(n-1)\left(2m - (2m/n)^2\right)},$$
 (28)

with equality holding if and only if $G = (n/2) K_2$, or $G = K_n$, or G is a strongly regular graph with parameters (n, k, a, a), where

$$k = 2m/n$$
, and $a = (k^2 - k)/(n-1)$.

Recall the following definition (see, e.g., [4], p. 144):

Definition 2.38. A strongly regular graph with parameters (n, k, a, a) is called a **design** graph.

Design graphs are quite rare, and since $(k^2 - k) / (n - 1) = a \ge 1$, for every k, there are finitely many design graphs of order n and degree k. Therefore, if m is a slowly growing function of n, equality in (28) does not hold if n is sufficiently large. This fact leads to the following problem:

Problem 2.39. Let $C \geq 1$. For all sufficiently large n, find the maximum $||G||_*$ if G is a graph of order n with at most Cn edges.

Further, recall that Koolen and Moulton deduced inequality (28) from a more general statement: If λ is the largest eigenvalue of G, then

$$||G||_* \le \lambda + \sqrt{(n-1)(2m-\lambda^2)},$$
 (29)

with equality if and only if $\sigma_2(G) = \cdots = \sigma_n(G)$.

The condition $\sigma_2(G) = \cdots = \sigma_n(G)$ is quite strong, but is hard to restate in non-spectral graph terms.

Suppose that a graph G of order n satisfies the condition $\sigma_2(G) = \cdots = \sigma_n(G)$. Clearly the eigenvalues $\lambda_2(G), \ldots, \lambda_n(G)$ take only two values, and so G is a graph with at most three eigenvalues. If G is regular, then either $G = (n/2) K_2$, or $G = K_n$, or G is a design graph.

If G is not regular and is disconnected, then $G = K_{n-2r} + rK_2$. We thus arrive at the following problem:

Problem 2.40. Give a constructive characterization of all connected irregular graphs G of order n with $|\lambda_2(G)| = \cdots = |\lambda_n(G)|$.

Given the problems listed above, one might predict that the real difficulties in the study of graph energy are still ahead of us.

3. The Ky Fan norms

In this section we survey some results on the Ky Fan norms of graphs and matrices, given in [11,33,34,36,37]. The main topic we are interested in is the maximal Ky Fan k-norm of graphs of given order. More precisely, define the function $\xi_k(n)$ as

$$\xi_{k}\left(n\right):=\max\left\{ \left\Vert G\right\Vert _{\left[k\right]}:G\text{ is a graph of order }n\right\} ,$$

and consider the following natural problem:

Problem 3.1. For all $n \geq k \geq 2$, find or approximate $\xi_k(n)$.

To begin with, following the approach of [28], it is not hard to find the asymptotics of $\xi_k(n)$:

Proposition 3.2. For every fixed positive integer k, the limit $\xi_k = \lim_{n \to \infty} \xi_k(n) / n$ exists.

Note that the maximal energy, i.e., the maximal Ky Fan n-norm, is of order $n^{3/2}$, whereas, for a fixed positive integer k, the maximal Ky Fan k-norm of an n vertex graph is linear in n. However, this fact does not make the solution of Problem 3.1 any easier.

It turns out that finding ξ_k (n) is hard for any $k \geq 2$, and even finding ξ_k is challenging; in particular, ξ_2 is not known yet, despite intensive research. Recall that in [11], Gregory, Hershkowitz and Kirkland asked what is the maximal value of the spread of a graph of order n, that is to say, what is

$$\max_{v(G)=n} \lambda_1(G) - \lambda_n(G).$$

This problem is still open, and even an asymptotic solution is not known, but in [33] it was shown that finding the maximum spread of a graph of order n is equivalent to finding $\xi_2(n)$.

It turns out that the study of maximal Ky Fan norms of matrices yields new insights into Hadamard matrices and partial Hadamard matrices. In Section 3.1 we give several matrix results, and deduce an upper bound on $\xi_k(n)$.

To find matching lower bounds, in Section 3.2 we discuss a class of matrices, which have been introduced in [36]. These matrices generalize symmetric Hadamard matrices, and provide infinite families of exact and approximate solutions to Problem 3.1, presented in Section 3.3.

In Section 3.4 we study Nordhaus–Gaddum problems for the Ky Fan norms of graphs and matrices, and give several tight bounds.

Finally, in Section 3.5, we study relations of Ky Fan norms to the chromatic number and the clique number of graphs.

3.1. Maximal Ky Fan norms of matrices

Applying the AM-QM inequality to the sum of the k largest singular values and using (7), we obtain the following theorem:

Theorem 3.3. Let $n \geq m \geq 2$ and $m \geq k \geq 1$. If $A \in M_{m,n}$, then

$$||A||_{[k]} \le \sqrt{k} ||A||_2.$$
 (30)

Equality holds if and only if A has exactly k nonzero singular values, which are equal.

It seems difficult to give a constructive characterization of all matrices that force equality in (30), since the given condition is exact, but is too general for constructive characterization. Thus, we give just one construction, showing the great diversity of this class:

Let $q \geq k$ and let B be a $k \times q$ matrix whose rows are pairwise orthogonal vectors of l_2 -norm equal to l. Since $BB^* = l^2I_k$, we see that all k singular values of B are equal to l. Now, choose arbitrary $r \geq 1$ and $s \geq 1$, and set $A := B \otimes J_{r,s}$. Obviously, A has exactly k nonzero singular values, which are equal, and so $||A||_{[k]} = \sqrt{k} ||A||_2$.

Further, the inequality $\|A\|_2 \leq \sqrt{mn} \|A\|_{\max}$ implies the following corollary:

Corollary 3.4. Let $n \geq m \geq k \geq 2$ and $A \in M_{m,n}$. If $||A||_{\max} \leq 1$, then

$$||A||_{[k]} \le \sqrt{kmn}.\tag{31}$$

Equality holds in (31) if and only if all entries of A have modulus 1, and A has exactly k nonzero singular values, which are equal to $\sqrt{mn/k}$.

Here is a general construction of matrices that force equality in (31): choose arbitrary $r \geq 1$, $s \geq 1$, $q \geq k$, let B be a $k \times q$ partial Hadamard matrix, and set $A := B \otimes J_{r,s}$. Since A has exactly k nonzero singular values, and they are equal, and since the entries of A are of modulus 1, we have $||A||_{[k]} = \sqrt{k} ||A||_2 = \sqrt{kmn}$, thus A forces equality in (31).

Although the upper bounds given in Theorem 3.3 and Corollary 3.4 are as good as one can get, for nonnegative matrices they can be improved.

Theorem 3.5. Let $n \ge m \ge k \ge 2$. If A is an $m \times n$ nonnegative matrix with $||A||_{\max} \le 1$, then

$$||A||_{[k]} \le \frac{\sqrt{kmn}}{2} + \frac{\sqrt{mn}}{2}.$$
 (32)

Equality holds in (32) if and only if the matrix $2A - J_{m,n}$ is a regular (-1,1)-matrix, with row sums equal to n/\sqrt{k} , and with exactly k nonzero singular values, which are equal to $\sqrt{mn/k}$.

Proof. Let $H := 2A - J_{m,n}$ and note that $||H||_{\max} \leq 1$. First, the AM-QM inequality implies that

$$||H||_{[k]} = \sigma_1(H) + \dots + \sigma_k(H) \le \sqrt{k \left(\sigma_1^2(H) + \dots + \sigma_k^2(H)\right)}$$

$$\le \sqrt{k \left(\sigma_1^2(H) + \dots + \sigma_n^2(H)\right)} = \sqrt{k} ||H||_2$$

$$< \sqrt{kmn}.$$

Hence, the triangle inequality implies that

$$||2A||_{[k]} = ||H + J_{m,n}||_{[k]} \le ||H||_{[k]} + ||J_{m,n}||_{[k]} \le \sqrt{kmn} + \sqrt{mn},$$

proving (32).

Now, suppose that a matrix A satisfies the premises and forces equality in (32), and let $H := 2A - J_{m,n}$. Obviously $||H||_2 = \sqrt{mn}$, and so H is a (-1,1)-matrix with

$$\sigma_1(H) = \cdots = \sigma_k(H) = \sqrt{mn/k}$$
 and $\sigma_i(H) = 0$ for $i > k$.

It remains to show that H is regular and calculate its row sums. Indeed, for every i = 2, ..., n, Weyl's inequality (1) implies that

$$\sigma_i(2A) \le \sigma_{i-1}(H) + \sigma_2(J_{m,n}) = \sqrt{mn/k}.$$

Since equality holds in (32), it follows that

$$\sigma_1(2A) \ge \sqrt{kmn} + \sqrt{mn} - (k-1)\sqrt{mn/k} = \sqrt{mn/k} + \sqrt{mn}$$
$$= \sigma_1(H) + \sigma_1(J_{m,n}).$$

On the other hand, letting $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^m$ be unit singular vectors to $\sigma_1(2A)$, we see that

$$\sigma_{1}(2A) = \langle 2A\mathbf{x}, \mathbf{y} \rangle = \langle H\mathbf{x}, \mathbf{y} \rangle + \langle J_{n}\mathbf{x}, \mathbf{y} \rangle \le \sigma_{1}(H) + \sigma_{1}(J_{n}). \tag{33}$$

Therefore, equality holds in (33), and so \mathbf{x} and \mathbf{y} are singular vectors to $\sigma_1(H)$ and to $\sigma_1(J_{m,n})$ as well; hence, $\mathbf{x} = n^{-1/2}\mathbf{j}_n$ and $\mathbf{y} = m^{-1/2}\mathbf{j}_m$. Thus, H is regular and its row sums are equal to

$$\frac{1}{m} \langle H \mathbf{j}_n, \mathbf{j}_m \rangle = \frac{1}{m} \sqrt{nm} \langle H \mathbf{x}, \mathbf{y} \rangle = \sqrt{\frac{n}{m}} \sigma_1(H) = \sqrt{\frac{n}{m}} \sqrt{mn/k} = n/\sqrt{k},$$

as claimed.

We omit the proof that the given conditions on A force equality in (32). \Box

The class $\mathbb{R}_{m,n}(k)$ of regular (-1,1)-matrices, with row sums equal to n/\sqrt{k} and with k nonzero and equal singular values, seems quite remarkable. Note that $\mathbb{R}_{m,n}(k)$ consists of matrices of rank k, and some of them are Kronecker products of partial Hadamard matrices. Yet, in many cases $\mathbb{R}_{m,n}(k)$ contains matrices that are not Kronecker products of partial Hadamard matrices. The complete characterization of $\mathbb{R}_{m,n}(k)$ is an open problem.

For graphs we get a straightforward corollary of Theorem 3.5:

Theorem 3.6. If $n \ge k \ge 2$, and G is a graph of order n with adjacency matrix A, then

$$||G||_{[k]} \le \frac{n\sqrt{k}}{2} + \frac{n}{2}.$$
 (34)

Equality holds in (34) if and only if $2A - J_n$ is a regular, symmetric (-1,1)-matrix, with -1 along the diagonal, with row sums equal to n/\sqrt{k} , and with exactly k nonzero singular values, which are equal to n/\sqrt{k} .

Clearly, Theorem 3.6 is a far reaching generalization of the Koolen and Moulton upper bound (2). The condition for equality, however, is different, and we can say more about it. To this end, we need some preliminary work, which was recently reported in [36], and which we state in the following section. For the missing proofs the reader is referred to [36].

3.2. An extension of symmetric Hadamard matrices

To study maximal Ky Fan norms of graphs we need symmetric (-1, 1)-matrices whose nonzero singular values are equal. Such matrices have distinctive properties and deserve close attention, for they extend symmetric Hadamard matrices in a nontrivial way.

Thus, write n(A) for the order of a square matrix A, and let \mathbb{S}_k be the set of symmetric (-1,1)-matrices with $\sigma_k(A) = n(A)/\sqrt{k}$.

First, note that if an $n \times n$ matrix A, with all entries of modulus 1, satisfies $\sigma_k(A) = n/\sqrt{k}$, then

$$\sigma_1(A) = \cdots = \sigma_k(A) = n/\sqrt{k}$$
 and $\sigma_i(A) = 0$ for $k < i \le n$.

Further, if $A \in \mathbb{S}_k$, and if a matrix B can be obtained by permutations or negations performed simultaneously on the rows and columns of A, then $B \in \mathbb{S}_k$ as well; the reason is that A and B have the same singular values.

For reader's sake, we list six basic properties of \mathbb{S}_k , whose proofs are omitted:

- (1) If $A \in \mathbb{S}_k$, then $-A \in \mathbb{S}_k$.
- (2) If A is a symmetric (-1,1)-matrix of rank 1, then $A \in \mathbb{S}_1$; thus, $J_n \in \mathbb{S}_1$.
- (3) If H is a symmetric Hadamard matrix of order k, then $H \in \mathbb{S}_k$; thus $\mathbb{S}_2 \neq \emptyset$.

- (4) If $A \in \mathbb{S}_k$ and $B \in \mathbb{S}_l$, then $A \otimes B \in \mathbb{S}_{kl}$; hence, if $\mathbb{S}_k \neq \emptyset$, then $\mathbb{S}_{2k} \neq \emptyset$.
- (5) If $A \in \mathbb{S}_k$, then $A \otimes J_n \in \mathbb{S}_k$ for any $n \geq 1$; hence, if $\mathbb{S}_k \neq \emptyset$, then \mathbb{S}_k is infinite.
- (6) If $\mathbb{S}_k \neq \emptyset$, then \mathbb{S}_k contains matrices with all row sums equal to zero.

Using Properties (1)–(6), one can show that \mathbb{S}_k contains matrices with some special properties, as in the following proposition:

Proposition 3.7. If $A \in \mathbb{S}_k$, then there is a $B \in \mathbb{S}_{2k}$ with $\operatorname{tr} B = 0$, that is, B has exactly k positive and exactly k negative eigenvalues.

Indeed, set

$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$

and let $B = K \otimes (H_2 \otimes A)$; obviously, $B \in \mathbb{S}_{2k}$ and tr B = 0.

Property (3) shows that the sets \mathbb{S}_k extend the class of symmetric Hadamard matrices. However, \mathbb{S}_k may also contain matrices that does not come from Hadamard matrices; e.g., we shall see that $\mathbb{S}_{s^2} \neq \emptyset$ for any natural number s.

The crucial question about \mathbb{S}_k is the following one:

Problem 3.8. For which k is \mathbb{S}_k nonempty?

As stated in Corollary 3.10 below, if k is odd and is not an exact square, then \mathbb{S}_k is empty. On the positive side, if k is the order of a symmetric Hadamard matrix, \mathbb{S}_k is nonempty, so there are infinitely many k for which \mathbb{S}_k is nonempty.

Here is a more definite assertion about \mathbb{S}_k :

Proposition 3.9. If $A \in \mathbb{S}_k$, then either k is an exact square, or $\operatorname{tr} A = 0$ and A has the same number of positive and negative eigenvalues.

Proof. Let $A = [a_{i,j}] \in \mathbb{S}_k$. Set $\lambda = \sigma_1(A)$, n = n(A), and let $\lambda_1 \geq \cdots \geq \lambda_n$ be the eigenvalues of A. We have

$$k\lambda^2 = \sum_{\lambda_i > 0} \lambda_i^2 + \sum_{\lambda_i < 0} \lambda_i^2 = \text{tr } A^2 = \sum_{i=1}^n \sum_{l=1}^n a_{i,j}^2 = n^2.$$

On the other hand, writing n_+ and n_- for the number of positive and negative eigenvalues of A, we see that

$$(n_+ - n_-)\lambda = \sum_{\lambda_i > 0} \lambda_i + \sum_{\lambda_i < 0} \lambda_i = \text{tr } A.$$

If tr A=0, then $n_+=n_-$, and so A has the same number of positive and negative eigenvalues. If tr $A\neq 0$, then λ is rational, implying that \sqrt{k} is rational, and so k is an exact square, completing the proof. \square

Corollary 3.10. If k is odd and \mathbb{S}_k is nonempty, then k is an exact square.

Let us note another corollary, which is a well-known fact about Hadamard matrices corresponding to graphs with maximal energy:

Corollary 3.11. If n is the order of a real symmetric Hadamard matrix with constant diagonal, then n is an exact square.

It seems important to determine if \mathbb{S}_k is empty for small k, say for $k \leq 10$. First, Corollary 3.10 implies that \mathbb{S}_k is empty for k = 3, 5, and 7. As shown in Theorems 3.13 and 3.14 below, if k is an exact square, then S_k is nonempty. Thus, in view of Properties (1)–(5), we see that \mathbb{S}_k is nonempty for k = 1, 2, 4, 8, and 9. The first unknown cases are k = 6 and k = 10.

Question 3.12. Is \mathbb{S}_6 empty?

Now, in Theorems 3.13 and 3.14 we state two constructions of symmetric (-1, 1)-matrices showing that \mathbb{S}_k is nonempty if k is an exact square. These constructions are proved in [36] by the Kharaghani method for Hadamard matrices [21], which apparently is applicable to more general (-1, 1)-matrices.

Theorem 3.13. For any integer $s \geq 2$, there are an integer $n \geq s$ and a symmetric (-1,1)-matrix B of order ns such that:

- (i) B has exactly s^2 nonzero eigenvalues, of which $\binom{s+1}{2}$ are equal to n, and $\binom{s}{2}$ are equal to -n;
 - (ii) the vector \mathbf{j}_{ns} is an eigenvector of B to the eigenvalue -n;
 - (iii) the diagonal entries of B are equal to 1.

Theorem 3.14. For any integer $s \geq 2$, there are an integer $n \geq s$ and a symmetric (-1,1)-matrix B of order ns such that:

- (i) B has exactly s^2 nonzero eigenvalues, of which $\binom{s+1}{2}-1$ are equal to n, and $\binom{s}{2}+1$ are equal to -n;
 - (ii) all row sums of B are equal to -n.

Note that Theorem 3.14 and Proposition 3.7 imply that for any natural number s, the classes \mathbb{S}_{s^2} and \mathbb{S}_{2s^2} are nonempty. To summarize, let us state some explicit solutions to Problem 3.8:

Proposition 3.15. Let s be a natural number and let p be a prime power, with $p = 1 \mod 4$. Then the classes \mathbb{S}_{s^2} , \mathbb{S}_{2s^2} , $\mathbb{S}_{2s^2(p+1)}$ and $\mathbb{S}_{4s^2(p+1)}$ are nonempty.

3.3. Maximal Ky Fan norms of graphs

Armed with the results of Section 3.2, we continue the study of $\xi_k(n)$. It turns out that if bound (34) is attained, then k is an exact square:

Theorem 3.16. If $n \ge k \ge 2$ and G is a graph of order n such that

$$||G||_{[k]} = \frac{n\sqrt{k}}{2} + \frac{n}{2},$$

then k is an exact square.

Proof. Suppose that G is a graph of order n with adjacency matrix A. For reader's sake, we breeze through part of the proof of Theorem 3.5.

The matrix $H := 2A - J_n$ is a symmetric (-1, 1)-matrix; hence the AM-QM inequality implies that

$$\sigma_{1}(H) + \dots + \sigma_{k}(H) \leq \sqrt{k \left(\sigma_{1}^{2}(H) + \dots + \sigma_{k}^{2}(H)\right)} \leq \sqrt{k \left(\sigma_{1}^{2}(H) + \dots + \sigma_{n}^{2}(H)\right)}$$
$$= \|H\|_{2} \sqrt{n} = n\sqrt{k}.$$

Therefore, the triangle inequality for the Ky Fan k-norm implies that

$$n\sqrt{k} + n = \|2A\|_{[k]} \le \|H\|_{[k]} + \|J_n\|_{[k]} \le n\sqrt{k} + n.$$

Thus, equalities hold throughout the above line, and so, H has k nonzero singular values, which are equal. We get

$$\sigma_k(H) = n/\sqrt{k},$$

implying that $H \in \mathbb{S}_k$. On the other hand, $\operatorname{tr} H = n \neq 0$, so H cannot have the same number of positive and negative eigenvalues, and Proposition 3.9 implies that k is an exact square. \square

The matrices constructed in Theorem 3.14 imply that the converse of Theorem 3.16 is true whenever k is an even square.

Theorem 3.17. Let $s \geq 2$ be an even positive integer. There exists a positive integer p, such that for any positive integer t, there is a graph G of order n = spt with

$$||G||_{[s^2]} = \frac{sn}{2} + \frac{n}{2}.$$

The proof of Theorem 3.17 can be found in [36]. This theorem is as good as one can get, but it is proved only for even s. However, if s is odd, $\xi_{s^2}(n)$ is just slightly below the upper bound (34), as implied by the following more general theorem:

Theorem 3.18. Suppose that \mathbb{S}_k contains a regular matrix B with nonzero row sums, say of order k. Then for any positive integer t, there is a graph G of order n = kt such that

$$||G||_{[k]} \ge \frac{n\sqrt{k}}{2} + \frac{n}{2} - k.$$
 (35)

The proof of Theorem 3.18 can be found in [36].

Note that Theorem 3.14 implies that for any integer $s \geq 2$, the set \mathbb{S}_{s^2} contains a regular matrix with nonzero row sums. Therefore, the premise of Theorem 3.18 holds for every $k = s^2$, where s is an integer and $s \geq 2$.

Dividing both sides of (35) by n and letting $n \to \infty$, we obtain the following corollary:

Corollary 3.19. If S_k contains a regular matrix B with nonzero row sums, then

$$\xi_k = \frac{\sqrt{k}}{2} + \frac{1}{2}.$$

Therefore, $\xi_4 = 3/2$, $\xi_9 = 2$, $\xi_{16} = 5/2$, $\xi_{25} = 3$, etc.

Since Theorem 3.16 does not shed any light on the case of non-square k, we state the following straightforward conjecture:

Conjecture 3.20. There exist infinitely many positive integers k such that

$$\xi_k < \frac{\sqrt{k}}{2} + \frac{1}{2}.$$

We end up this section with the easy asymptotics

$$\frac{\sqrt{k}}{2} \le \xi_k \le \frac{\sqrt{k}}{2} + \frac{1}{2}.$$

3.4. Nordhaus-Gaddum problems for Ky Fan norms

In this section we extend some results from Section 2.4 to Ky Fan norms of rectangular nonnegative matrices. Most of these results were proved in [38], but some new developments are presented here for the first time, so their proofs are given in full.

Theorem 3.21. If $n \ge m \ge k \ge 2$ and A is an $m \times n$ nonnegative matrix with $||A||_{\max} \le 1$, then

$$||A||_{[k]} + ||J_{m,n} - A||_{[k]} \le \sqrt{(k-1)mn} + \sqrt{mn}.$$
 (36)

Equality holds if only if A is a regular (0,1)-matrix such that

$$\sigma_1(A) = \sigma_1(\overline{A}) = \frac{\sqrt{mn}}{2}$$

and

$$\sigma_2(A) = \dots = \sigma_k(A) = \sigma_2(\overline{A}) = \dots = \sigma_k(\overline{A}) = \frac{1}{2}\sqrt{\frac{mn}{k-1}}.$$
 (37)

Proof. Set for short $\overline{A} = J_{m,n} - A$. Following a familiar path, we see that

$$\sigma_{1}(A) + \sigma_{1}(\overline{A}) + \sum_{i=2}^{k} \left(\sigma_{i}(A) + \sigma_{i}(\overline{A})\right)$$

$$\leq \sigma_{1}(A) + \sigma_{1}(\overline{A}) + \sqrt{2(k-1)\sum_{i=2}^{k} \left(\sigma_{i}^{2}(A) + \sigma_{i}^{2}(\overline{A})\right)}$$

$$\leq \sigma_{1}(A) + \sigma_{1}(\overline{A}) + \sqrt{2(k-1)\left(\left\|A\right\|_{2}^{2} + \left\|\overline{A}\right\|_{2}^{2} - \sigma_{1}^{2}(A) - \sigma_{1}^{2}(\overline{A})\right)}$$

$$\leq \sigma_{1}(A) + \sigma_{1}(\overline{A}) + \sqrt{2(k-1)\left(mn - \frac{(\sigma_{1}(A) + \sigma_{1}(\overline{A}))^{2}}{2}\right)}.$$

$$(38)$$

Since the function

$$f(x) = x + \sqrt{2(k-1)(mn - x^2/2)}$$

is decreasing in x for $x \ge \sqrt{mn}$, and also

$$\sigma_{1}(A) + \sigma_{1}(\overline{A}) \ge \frac{1}{\sqrt{mn}} \langle A\mathbf{j}_{n}, \mathbf{j}_{m} \rangle + \frac{1}{\sqrt{mn}} \langle \overline{A}\mathbf{j}_{n}, \mathbf{j}_{m} \rangle = \frac{1}{\sqrt{mn}} \langle J_{m,n}\mathbf{j}_{n}, \mathbf{j}_{m} \rangle = \sqrt{mn},$$
(39)

we see that

$$||A||_* + ||\overline{A}||_* \le \sqrt{(k-1)mn} + \sqrt{mn},$$

completing the proof of (36).

If equality holds in (36), then $||A||_2^2 + ||\overline{A}||_2^2 = mn$, which means that A is a (0,1)-matrix, and so is \overline{A} . Further,

$$\sigma_1^2(A) + \sigma_1^2(\overline{A}) = (\sigma_1(A) + \sigma_1(\overline{A}))^2/2 = \frac{mn}{2},$$

which means that $\sigma_1(A) = \sigma_1(\overline{A}) = \sqrt{mn}/2$. Hence equalities hold throughout (39), and so A is regular.

Finally, the AM–QM inequality applied in (38) is equality precisely if

$$\sigma_2(A) = \cdots = \sigma_k(A) = \sigma_2(\overline{A}) = \cdots = \sigma_k(\overline{A}),$$

and since

$$\sigma_2^2(A) + \dots + \sigma_k^2(A) + \sigma_2^2(\overline{A}) + \dots + \sigma_k^2(\overline{A}) = \frac{mn}{2},$$

we obtain (37).

We omit the proof that the given conditions on A force equality in (36). Theorem 3.21 is proved. \Box

It seems hard to give a constructive description of all matrices A forcing equality in (36), so we raise the following problem:

Problem 3.22. Let $n \ge m \ge k \ge 2$. Find a constructive description of all $m \times n$ nonnegative matrices A with $||A||_{\max} \le 1$ such that

$$||A||_{[k]} + ||J_{m,n} - A||_{[k]} = \sqrt{(k-1)mn} + \sqrt{mn}.$$

Nevertheless, here is a construction showing that (36) is exact in a rich set of cases.

Theorem 3.23. Let $t \ge k-1 \ge 2$, and let B be a $(k-1) \times t$ partial Hadamard matrix. Let $p, q \ge 1$ be arbitrary integers and set m = 2(k-1)p and n = 2tq. Then, there exists a (0,1)-matrix A of size $m \times n$ such that

$$||A||_{[k]} + ||J_{m,n} - A||_{[k]} = \sqrt{(k-1)mn} + \sqrt{mn}.$$

Proof. Set

$$H = \begin{bmatrix} B & -B \\ -B & B \end{bmatrix}$$

and let

$$A = \frac{1}{2} \left((H \otimes J_{p,q}) + J_{m,n} \right).$$

Obviously, A is a (0,1)-matrix of size $m \times n$. Our goal is to show that $\sigma_1(A) = \sqrt{mn}/2$ and that

$$\sigma_2(A) = \dots = \sigma_k(A) = \frac{1}{2} \sqrt{\frac{mn}{k-1}}.$$

Recall that B has k-1 nonzero singular values and they are equal to $t/\sqrt{k-1}$. Hence, H has k-1 nonzero singular values, which are equal to $2t/\sqrt{k-1}$, and so, $H\otimes J_{p,q}$ has k-1 nonzero singular values, which are equal to

$$2t\sqrt{\frac{pq}{k-1}}=\sqrt{\frac{2tp2tq}{k-1}}=\sqrt{\frac{mn}{k-1}}.$$

Clearly, the row and column sums of H are 0, and thus 0 is a singular value of H with singular vectors $(2(k-1))^{-1/2}\mathbf{j}_{2(k-1)}$ and $(2t)^{-1/2}\mathbf{j}_{2t}$; hence, 0 is a singular value of $H \otimes J_{p,q}$ with singular vectors $m^{-1/2}\mathbf{j}_m$ and $n^{-1/2}\mathbf{j}_n$. Since the unique nonzero singular value of $J_{m,n}$ is \sqrt{mn} , with singular vectors $m^{-1/2}\mathbf{j}_m$ and $n^{-1/2}\mathbf{j}_n$, it is obvious that

$$\sigma_1(A) = \frac{\sqrt{mn}}{2}$$
 and $\sigma_2(A) = \cdots = \sigma_k(A) = \frac{1}{2}\sqrt{\frac{mn}{k-1}}$.

Hence,

$$||A||_{[k]} = \frac{\sqrt{mn}}{2} + \frac{1}{2}\sqrt{\frac{mn}{k-1}}(k-1) = \frac{\sqrt{(k-1)\,mn}}{2} + \frac{\sqrt{mn}}{2}.$$

On the other hand,

$$J_{m,n} - A = \frac{1}{2} \left(\left(-H \otimes J_{p,q} \right) + J_{m,n} \right),\,$$

and so $J_{m,n} - A$ has the same singular values as A, because $-B \in \mathbb{S}_{k-1}$ as well. This completes the proof of Theorem 3.23. \square

Note that Theorems 3.21 and 3.23 are matrix results, easier than the corresponding results for graphs. To get a meaningful statement for graphs, we propose a matrix problem, which probably can be solved following the proof of Theorem 2.28:

Problem 3.24. Let $n \ge k \ge 2$ and let A be a $n \times n$ symmetric nonnegative matrix with $||A||_{\max} \le 1$ and with zero diagonal. Find the maximum of

$$||A||_{[k]} + ||J_{m,n} - I_n - A||_{[k]}$$
.

Finally, note that Theorem 3.21 is stated and proved for $k \geq 2$. As it turns out, the Ky Fan 1 norm (i.e., the operator norm) is completely different (for a proof see [38]).

Theorem 3.25. If A is an $m \times n$ nonnegative matrix with $||A||_{\max} \leq 1$, then,

$$\sigma_1(A) + \sigma_1(J_{m,n} - A) \le \sqrt{2mn},\tag{40}$$

with equality holding if and only if mn is even, and A is a (0,1)-matrix with precisely mn/2 ones that are contained either in n/2 columns or in m/2 rows.

3.5. Ky Fan norms and some graph parameters

This section contains a few relations of Ky Fan norms with basic graph parameters, which lead to some challenging open problems.

Recall the well-known result of Caporossi, Cvetković, Gutman, and Hansen [6]:

If G is a graph, then

$$||G||_{\pi} > 2\lambda_1(G), \tag{41}$$

with equality holding if and only if G is a complete multipartite graph with possibly some isolated vertices.

We shall uncover the role of the chromatic number in (41): Let G be a graph of order n and chromatic number χ . Recall the famous inequality of Hoffman [19]

$$\lambda_1(G) \le |\lambda_n(G)| + \dots + |\lambda_{n-\gamma+2}(G)|, \tag{42}$$

which obviously implies that

$$\lambda_1(G) \leq \sigma_2(G) + \cdots + \sigma_{\chi}(G)$$
.

Thus, Hoffman's inequality (42) strengthens (41) as follows:

Theorem 3.26. If G is a graph with chromatic number $\chi \geq 2$, then

$$||G||_{[\gamma]} \ge 2\lambda_1(G). \tag{43}$$

Note that if G is a complete χ -partite graph with possibly some isolated vertices, then equality holds in (43). However, there are many other cases of equality some of which are rather complicated. Clearly, if equality holds in (43), then equality holds in (42), but the converse is not obvious. Thus, we raise the following problem:

Problem 3.27. Which graphs G satisfy the equality $||G||_{[\chi]} = 2\lambda_1(G)$?

In contrast to Theorem 3.26, for bipartite graphs we have

$$||G||_{[2]} = 2\lambda_1(G) \le 2\sqrt{\lfloor n^2/4 \rfloor}.$$

A similar inequality for r-partite graphs seems unknown, so we raise the following problem:

Problem 3.28. What is the maximum of $||G||_{[\chi]}$ of an χ -chromatic graph of order n.

Next, recall that in [11], Gregory, Hershkowitz and Kirkland proved the following theorem:

Theorem 3.29. If G is a graph with m edges and largest eigenvalue λ , then

$$||G||_{[2]} \le \lambda + \sqrt{2m - \lambda^2} \le 2\sqrt{m}. \tag{44}$$

Equality holds in (44) if and only if G is a complete bipartite graph with possibly some isolated vertices.

As the authors of [11] note: if $m > \lfloor n^2/4 \rfloor$, bound (44) is never attained. Thus, let us reiterate one of the problems in [11]:

Problem 3.30. If G is a graph of order n, with m edges, how large can $||G||_{[2]}$ be?

Further, note that Mantel's theorem [26] gives the following immediate corollary of inequality (44).

Corollary 3.31. If G is a triangle-free graph of order n, then

$$||G||_{[2]} < 2\sqrt{\lfloor n^2/4 \rfloor},$$

unless $G = K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

The extension of this statement to K_{r+1} -free graphs (graphs without a complete subgraph of order r+1) for $r \geq 3$ is nowhere in sight. We state two versions of such a problem:

Problem 3.32. If $r \geq 3$ and G is a K_{r+1} -free graph with m edges, how large can $||G||_{[r]}$ be?

Problem 3.33. If $r \geq 3$ and G is a K_{r+1} -free graph of order n, how large can $||G||_{[r]}$ be?

Finally, it is interesting to study the following problems, which are typical for the study of graph energy.

Problem 3.34. Let $k \geq 2$ and G let be a connected graph of sufficiently large order n. Is it true that

$$||G||_{[k]} \ge ||P_n||_{[k]}$$
,

where P_n is the path of order n?

Problem 3.35. Let $k \geq 2$ and T be a tree of sufficiently large order n. How large $||T||_{[k]}$ can be?

4. The Schatten norms

This section is dedicated to the Schatten norms of graphs and matrices. Unlike the somewhat choppy Ky Fan k-norms, the Schatten p-norms are rather smooth; thus, many results on graph energy seamlessly extend to Schatten norms.

Since the parameter p in the Schatten p-norm may be any real number in the interval $[1, \infty)$, some new problems arise, for which graph energy provides no clues at all. Such problems are discussed in the opening Section 4.1, with the rest of Section 4 dedicated to more traditional topics.

In Section 4.2, we discuss extremal Schatten p-norms of matrices and their relations to Hadamard matrices. We show that the use of p allows to obtain lower and upper bounds with the same argument; in particular, two bound converters similar to Proposition 2.7 are obtained with the same proof.

In Section 4.3, we discuss bounds on Schatten p-norms of graphs, most of which come from matrix bounds, combined with some results about graphs. Once more it is shown that, depending on p, lower bounds become upper, and vice versa.

Section 4.4 contributes to the popular topic of spectral moments in graph energy. We shall show that Hölder's inequality and Schatten norms provide a very convenient setup for this topic, and shall extend several known results.

In Section 4.5, we give a straightforward generalization of the results on the trace norms of r-partite graphs and matrices stated in Section 2.3, this time with proofs. As before, Kronecker products of conference and Hadamard matrices provide the tightest known bounds.

In the brief Section 4.6 we shall raise several question about extremal Schatten norms of trees.

Finally, in Section 4.7, we discuss the Schatten p-norm of almost all graphs, which turn to be as highly concentrated as the energy.

4.1. The Schatten p-norm as a function of p

As mentioned above, Schatten p-norms open a new direction of research, with no roots in graph energy. To elaborate this point, given a graph G, define the function $f_G(x)$ for any $x \ge 1$ as

$$f_G\left(x\right) := \left\|G\right\|_x.$$

The energy of G is just $f_G(1)$, but the function $f_G(x)$ delivers much more. Thus, let us give some analytic statements, with no analogs in the study of graph energy.

Proposition 4.1. For any graph G, the function $f_G(x)$ is differentiable in x.

The proof of this proposition is simple calculus, so we omit it. Here is another fact:

Proposition 4.2. For any nonempty graph G, the function $f_G(x)$ is decreasing in x.

Proof. Indeed, let G be graph of order n with singular values $\sigma_1, \ldots, \sigma_n$. If x < y, then

$$f_{G}(x) = \sigma_{1} \left(1 + \left(\frac{\sigma_{2}}{\sigma_{1}} \right)^{x} + \dots + \left(\frac{\sigma_{n}}{\sigma_{1}} \right)^{x} \right)^{1/x} \ge \sigma_{1} \left(1 + \left(\frac{\sigma_{2}}{\sigma_{1}} \right)^{y} + \dots + \left(\frac{\sigma_{n}}{\sigma_{1}} \right)^{y} \right)^{1/x}$$

$$> \sigma_{1} \left(1 + \left(\frac{\sigma_{2}}{\sigma_{1}} \right)^{y} + \dots + \left(\frac{\sigma_{n}}{\sigma_{1}} \right)^{y} \right)^{1/y}$$

$$= f_{G}(y). \quad \Box$$

Using calculus, we obtain another property of $f_G(x)$:

Proposition 4.3. For any graph G, the limit $\lim_{x\to\infty} f_G(x)$ exists and is equal to $\lambda_1(G)$.

Propositions 4.2 and 4.3 imply that the range of $f_G(x)$ is the interval $(\lambda_1(G), ||G||_*]$. Next, we restate a basic and well-known fact in spectral graph theory:

Proposition 4.4. If G is a graph with m edges, then $f_G(2) = \sqrt{2m}$. Furthermore, for any k > 1, the number of closed walks of length 2k of a graph G is equal to $(f_G(2k))^{2k}/4k$.

Given that the number of edges and so many other graph parameters can be read from the function $f_G(2)$, it is natural to ask the following question:

Question 4.5. Which graph properties can be determined from the function $f_G(x)$ alone?

Let us note that the order of a graph G cannot be determined from $f_G(x)$, because adding or removing isolated vertices does not change $f_G(x)$. Here is another example to the same effect, for connected graphs: let $F := K_{n,n}$ and $H := K_{1,n^2}$; obviously, $f_F(x) = f_H(x) = n2^{1/x}$, but v(F) = 2n and $v(H) = n^2 + 1$.

Although we cannot infer the order of G from $f_G(x)$, we can find the singular spectrum of G, that is, the nonzero singular values of G together with their multiplicities.

Proposition 4.6. There is a procedure that calculates the nonzero singular values and their multiplicities of any graph G if the function $f_G(x)$ is given.

Proof. Clearly we can find $\sigma_1(G)$, for $\sigma_1(G) = \lambda_1(G) = \lim_{x\to\infty} f_G(x)$. Now, the multiplicity k_1 of $\sigma_1(G)$ clearly is equal to

$$\lim_{x \to \infty} \frac{f_G^x(x)}{\sigma_1^x(G)}.$$

Next, we see that

$$\lim_{x \to \infty} \left(f_G^x(x) - k_1 \sigma_1^x(G) \right)^{1/x} = \sigma_2(G),$$

and if $\sigma_2(G) \neq 0$, we can determine the multiplicity of $\sigma_2(G)$ as

$$\lim_{x \to \infty} \frac{f_G^x(x) - k_1 \sigma_1^x(G)}{\sigma_2^x(G)}.$$

Iterating this argument, we obtain all nonzero singular values of G, along with their multiplicities. \square

Put in a different way, $f_G(x)$ carries the same information as the singular spectrum of G. Obviously, cospectral graphs have the same singular spectrum, but the converse may not be true. On the other hand, any two graphs with the same singular spectrum are coenergetic, but the converse may not be true. Hence, $f_G(x)$ introduces a new type of equivalence among graphs, which needs further study.

Let us spell out the relevant definition and raise a problem.

Definition 4.7. Two graphs G and H are called **singularly cospectral** if they have the same nonzero singular values with the same multiplicities.

Problem 4.8. Find necessary and sufficient conditions two graphs to be singularly cospectral.

Clearly Proposition 4.6 implies that two graphs G and H are singularly cospectral if and only if $f_G(x) = f_H(x)$.

4.2. Bounds on the Schatten p-norm of matrices

We start with a general inequality for the Schatten norms of arbitrary matrices in $M_{m,n}$.

Theorem 4.9. Let $n \geq m \geq 2$ and $q > p \geq 1$. If $A \in M_{m,n}$, then

$$m^{-1/p} \|A\|_p \le m^{-1/q} \|A\|_q$$
 (45)

If $A \neq 0$, equality holds in (45) if and only if the following equivalent conditions hold:

- (i) A has m nonzero singular values which are equal;
- (ii) AA^* is a scalar multiple of the identity matrix I_m .

Proof. Inequality (45) follows by applying the PM inequality to the singular values of A; so it remains to prove the characterization of the matrices that force equality in (45). Let $A \in M_{m,n}$. If A satisfies either (i) or (ii), then obviously A forces equality in (45).

Now, suppose that A forces equality in (45). Clearly, the condition for equality in the PM inequality implies (i). To complete the proof, we shall deduce (ii) from (i) using the idea of the proof of Proposition 2.1.

To begin with, note that the matrix $B := AA^*$ is an $m \times m$ Hermitian matrix, with m equal eigenvalues, which are the squares of the singular eigenvalues of A. Let $B = [b_{i,j}]$ and fix two distinct $s, t \in [m]$. The 2×2 principal submatrix

$$B' = \begin{bmatrix} b_{s,s} & b_{s,t} \\ b_{t,s} & b_{t,t} \end{bmatrix}$$

satisfies $b_{s,s} = \overline{b_{s,s}}$, $b_{t,t} = \overline{b_{t,t}}$, $b_{s,t} = \overline{b_{t,s}}$, and so the eigenvalues of B' are

$$\lambda_{1}(B') = \frac{b_{s,s} + b_{t,t} + \sqrt{(b_{s,s} - b_{t,t})^{2} + 4|b_{s,t}|^{2}}}{2},$$
$$\lambda_{2}(B') = \frac{b_{s,s} + b_{t,t} - \sqrt{(b_{s,s} - b_{t,t})^{2} + 4|b_{s,t}|^{2}}}{2}.$$

On the other hand, Cauchy's interlacing theorem implies that

$$\lambda_1(B) \ge \lambda_1(B') \ge \lambda_2(B') \ge \lambda_m(B)$$
,

which, in view of $\lambda_1(B) = \lambda_m(B)$, implies that $b_{s,s} = b_{t,t}$ and $b_{s,t} = b_{t,s} = 0$. Therefore, B has a constant diagonal and all its off-diagonal entries are zero. Hence, $B = aI_m$ for some a > 0, completing the proof of Theorem 4.9. \square

It is instructive to pair Theorem 4.9 with a similar lower bound on $\|A\|_p$.

Theorem 4.10. Let $n \geq m \geq 2$ and $q > p \geq 1$. If $A \in M_{m,n}$, then

$$||A||_p \ge ||A||_q \,. \tag{46}$$

Equality holds in (46) if and only if $\sigma_2(A) = 0$.

Proof. Let $A \in M_{m,n}$ and recall that

$$\sigma_1^p(A) + \dots + \sigma_m^p(A) = ||A||_p^p.$$
 (47)

To maximize $||A||_p$ subject to (47), note that q/p > 1, and so $x^{q/p}$ is a strictly convex function; hence, if x_1, \ldots, x_m are nonnegative real numbers, with $x_1 + \cdots + x_m = s > 0$, then

$$x_1^{q/p} + \dots + x_m^{q/p} \le s^{q/p},$$

with equality if and only if all but one of the numbers x_1, \ldots, x_m are zero.

In our case, letting

$$x_1 = \sigma_1^p(A), \dots, x_m = \sigma_m^p(A)$$
 and $s = ||A||_p^p$,

we see that

$$||A||_q^q = \sigma_1^q(A) + \dots + \sigma_m^q(A) = (\sigma_1^p(A))^{q/p} + \dots + (\sigma_m^p(A))^{q/p}$$

 $\leq ||A||_p^q,$

with equality if and only if $\sigma_1(A) = ||A||_p$ and $\sigma_2(A) = \cdots = \sigma_m(A) = 0$. \square

Next we shall explore some upper bounds on $\|A\|_p$. If we restrict $\|A\|_{\max}$, Theorems 4.9 and 4.10 imply absolute bounds on $\|A\|_p$. Note that these bounds and their cases of equality differ significantly for p < 2 and p > 2, so we state them in two separate theorems, whose proofs are omitted. The reasons for the difference between the cases p < 2 and p > 2 elude us.

Theorem 4.11. Let $n \ge m \ge 2$ and $2 > p \ge 1$. If $A \in M_{m,n}$ and $||A||_{\max} \le 1$, then

$$||A||_p \leq m^{1/p} n^{1/2}.$$

Equality holds if and only if A is a partial Hadamard matrix.

Theorem 4.12. Let $n \geq m \geq 2$ and p > 2. If $A \in M_{m,n}$ and $||A||_{max} \leq 1$, then

$$||A||_n \leq \sqrt{mn}$$
.

Equality holds in if and only if $\sigma_2(A) = 0$, and all entries of A are of modulus 1.

The triangle inequality for the Schatten norms implies neat bounds for nonnegative matrices as well. Unfortunately, these bounds are tight, but not sharp. Our first result is a generalization of (5):

Theorem 4.13. Let $n \ge m \ge 4$, $2 > p \ge 1$, and let A be an $m \times n$ nonnegative matrix. If $||A||_{\max} \le 1$, then

$$||A||_p \le \frac{m^{1/p} n^{1/2}}{2} + \frac{\sqrt{mn}}{2},$$
 (48)

If $2A - J_{m,n}$ is a regular partial Hadamard matrix, then

$$||A||_p \ge \frac{m^{1/p} n^{1/2}}{2}.$$

Proof. Suppose that A satisfies the premises of the theorem and let $H := 2A - J_{m,n}$. Obviously $||H||_{\max} \leq 1$ and the triangle inequality implies that

$$||2A||_p = ||H + J_n||_p \le ||H||_p + ||J_{m,n}||_p = ||H||_p + \sqrt{mn}.$$

Theorem 4.11 gives $||H||_p \le m^{1/p} n^{1/2}$ and (48) follows.

If H is a regular partial Hadamard matrix, then the singular values of 2A are \sqrt{n} with multiplicity m-1, and one singular value equal to $|\sqrt{nm} \pm \sqrt{n}|$. Since $m \geq 4$, it follows that all m nonzero singular values of A are at least \sqrt{n} and so

$$||A||_p \ge \frac{m^{1/p} n^{1/2}}{2},$$

completing the proof. \Box

The next statement complements Theorem 4.13 for p > 2, and in fact follows immediately from Theorem 4.12.

Corollary 4.14. Let $n \ge m \ge 2$, p > 2, and let A be an $m \times n$ nonnegative matrix. If $||A||_{\max} \le 1$, then

$$||A||_p \le \sqrt{mn}.$$

Equality holds if and only if $A = J_{m,n}$.

Theorems 4.9, 4.11, and 4.12 provide straightforward bounds, good for their simplicity, but quite rigid. However, in exchange for a somewhat complicated form, one can come up with more flexible inequalities, as the following one:

Proposition 4.15. Let $n \geq m \geq 2$ and $q > p \geq 1$. If $A \in M_{m,n}$, then

$$||A||_{p}^{p} \le \sigma_{1}^{p}(A) + (m-1)^{1-p/q} \left(||A||_{q}^{q} - \sigma_{1}^{q}(A) \right)^{p/q}.$$
(49)

Equality holds in (49) if and only if $\sigma_2(A) = \cdots = \sigma_m(A)$.

Proof. The PM inequality, applied to the numbers $\sigma_2(A), \ldots, \sigma_m(A)$, gives

$$(m-1)^{-1/p} \left(\|A\|_p^p - \sigma_1^p(A) \right)^{1/p} \le (m-1)^{-1/q} \left(\|A\|_q^q - \sigma_1^q(A) \right)^{1/q},$$

and inequality (49) follows, together with the condition for equality. \Box

Note that Proposition 4.15, just like Proposition 2.7, is a "bound generator". We can see that by repeating the argument after Proposition 2.7. Therefore, Proposition 4.15

can be used to convert lower bounds on $\sigma_1(A)$ into upper bounds on $||A||_p$. In particular, in [30] an infinite family of lower bounds on $\sigma_1(A)$ is given; hence, with some restrictions we may get an unlimited family of upper bounds on $||A||_p$. Here is one of them, which is based on the lower bound (11).

Proposition 4.16. Let $n \geq m \geq 2$, $q > p \geq 1$ and $A \in M_{m,n}$. If

$$\left|\sum\nolimits_{i,j}a_{ij}\right|\geq m^{1/2-1/q}n^{1/2}\left\|A\right\|_{q},$$

then

$$||A||_{p}^{p} \leq (mn)^{-p/2} \left| \sum_{i,j} a_{ij} \right|^{p} + (m-1)^{1-p/q} \left(||A||_{q}^{q} - (mn)^{-q/2} \left| \sum_{i,j} a_{ij} \right|^{q} \right)^{p/q}.$$

If equality holds in (12), then $\sigma_2(A) = \cdots = \sigma_m(A)$, the matrix A is regular and $\sigma_1(A) = (mn)^{-1/2} \left| \sum_{i,j} a_{ij} \right|$.

If A is nonnegative, then equality holds in (12) if and only if A is regular and $\sigma_2(A) = \cdots = \sigma_m(A)$.

We now turn to lower bounds on $||A||_p$. Theorems 4.10, and 4.12 provide straightforward and simple bounds, but in exchange for certain complication in form, we can obtain more flexible inequalities, as in the following proposition, which is a twin of Proposition 4.15:

Proposition 4.17. Let $n \geq m \geq 2$ and $p > q \geq 1$. If $A \in M_{m,n}$, then

$$||A||_p^p \ge \sigma_1^p(A) + (m-1)^{1-p/q} \left(||A||_q^q - \sigma_1^q(A) \right)^{p/q}.$$

Equality holds if and only if $\sigma_2(A) = \cdots = \sigma_m(A)$.

The proof of Proposition 4.17 is absolutely the same as the proof of Proposition 4.15. Note that Proposition 4.17, is also a "bound generator". The argument is the same as above. Hence, Proposition 4.17 can be used to convert lower bounds on $\sigma_1(A)$ into lower bounds on $||A||_p$. Here is a lower bound on $||A||_p$ obtained from the lower bound (11).

Proposition 4.18. Let $n \geq m \geq 2$, $p > q \geq 1$ and $A \in M_{m,n}$. If

$$\left| \sum\nolimits_{i,j} {{a_{ij}}} \right| \ge m^{1/2 - 1/q} n^{1/2} \left\| A \right\|_q,$$

then

$$||A||_{p}^{p} \ge (mn)^{-p/2} \left| \sum_{i,j} a_{ij} \right|^{p} + (m-1)^{1-p/q} \left(||A||_{q}^{q} - (mn)^{-q/2} \left| \sum_{i,j} a_{ij} \right|^{q} \right)^{p/q}.$$

If equality holds in (12), then $\sigma_2(A) = \cdots = \sigma_m(A)$, the matrix A is regular and $\sigma_1(A) = (mn)^{-1/2} \left| \sum_{i,j} a_{ij} \right|$.

If A is nonnegative, then equality holds in (12) if and only if A is regular and $\sigma_2(A) = \cdots = \sigma_m(A)$.

It seems particularly interesting to characterize nonnegative matrices forcing equality in Propositions 4.16 and 4.18, because we obtain a far reaching extension of design graphs.

Problem 4.19. Let $n \geq m \geq 2$. Give a constructive characterization of all regular nonnegative $m \times n$ matrices A with $\sigma_2(A) = \cdots = \sigma_m(A)$.

Finally, let us note a natural extension of the simple bound (15):

Proposition 4.20. If $2 > p \ge 1$ and A is a matrix with rank greater than 1, then

$$||A||_{p}^{p} \ge \sigma_{1}^{p}(A) + \frac{||A||_{2}^{2} - \sigma_{1}^{2}(A)}{\sigma_{2}^{2-p}(A)}$$
(50)

Equality holds if and only if all nonzero singular values of A other than $\sigma_1(A)$ are equal.

Proof. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the nonzero singular values of A. We see that

$$||A||_p^p = \sigma_1^p + \sigma_2^2 \sigma_2^{p-2} + \dots + \sigma_n^2 \sigma_n^{p-2}$$

$$\geq \sigma_1^p + \frac{\sigma_2^2}{\sigma_2^{2-p}} + \dots + \frac{\sigma_n^2}{\sigma_2^{2-p}} = \sigma_1^p + \frac{||A||_2^2 - \sigma_1^2}{\sigma_2^{2-p}},$$

and (50) follows.

4.3. Bounds on the Schatten p-norm of graphs

As mentioned above, usually results about graph energy extend to Schatten norms rather smoothly. The goal of this subsection is to demonstrate this fact on a few central results.

Let us start by restating Propositions 4.15 and 4.17 for graphs.

Corollary 4.21. If $q > p \ge 1$ and G is a graph of order n with largest eigenvalue λ , then

$$||G||_p^p \le \lambda^p + (m-1)^{1-p/q} (||G||_q^q - \lambda^q)^{p/q}.$$

Equality holds if and only if $\sigma_2(G) = \cdots = \sigma_n(G)$.

Corollary 4.22. If $p > q \ge 1$ and G is a graph of order n with largest eigenvalue λ , then

$$||G||_p^p \ge \lambda^p + (m-1)^{1-p/q} \left(||G||_q^q - \lambda^q\right)^{p/q}.$$

Equality holds if and only if $\sigma_2(G) = \cdots = \sigma_n(G)$.

Two remarks are in place here: First, let us reiterate that the condition $\sigma_2(G) = \cdots = \sigma_n(G)$, albeit exact, is not constructive, and we are again lead to Problem 4.19. Second, just like Propositions 4.15 and 4.17, Corollaries 4.21 and 4.22 are bound converters, even better ones because it is easier to find appropriate lower bounds for λ , which will produce upper or lower bounds on $\|G\|_p$. To simplify the presentation we focus exclusively on the pivotal case q=2, thereby making use of the equality $\|G\|_2^2=2e(G)$.

4.3.1. Upper bounds for $2 > p \ge 1$

For q = 2 Corollary 4.21 gives a practical and flexible bound:

Corollary 4.23. Let $2 > p \ge 1$. If G is a graph of order n and size m, with largest eigenvalue λ , then

$$||G||_p^p \le \lambda^p + (n-1)^{1-p/2} (2m - \lambda^2)^{p/2}.$$
 (51)

Equality holds in (51) if and only if $\sigma_2(G) = \cdots = \sigma_n(G)$.

Inequality (51) also is a "bound generator", which can convert lower bounds on λ into upper bounds on $\|G\|_p$. For example, the well-known inequality $\lambda \geq 2m/n$ yields a generalization of another bound of Koolen and Moulton [23]:

Proposition 4.24. If $2 > p \ge 1$, $m \ge n/2$, and G is a graph of order n and size m, then

$$||G||_p^p \le (2m/n)^p + (n-1)^{1-p/2} \left(2m - (2m/n)^2\right)^{p/2}.$$
 (52)

Equality holds if and only if G is either $(n/2) K_2$, or K_n , or a design graph.

However, inequality $\lambda \geq 2m/n$ is just one of the infinitely many lower bounds on λ in terms of walks, see [29] for details. Since these lower bounds are stronger than $\lambda \geq 2m/n$, they imply infinitely many upper bounds on $\|G\|_p$.

Next, we want an absolute bound on $||G||_p$ depending just on the order of G. We can use (52) and some calculus to get such a bound, but it will be very tangled. Instead, Theorem 4.13 provides a concise expression, which generalizes Koolen and Moulton's bound (2):

Theorem 4.25. If $2 > p \ge 1$ and G is a graph of order n with adjacency matrix A, then

$$||G||_p \le \frac{n^{1/p+1/2}}{2} + \frac{n}{2}. (53)$$

If G is a graph of maximal energy, then

$$||G||_p > \frac{n^{1/p+1/2}}{2}.$$

Note that bound (53) is never attained, but may be rather tight.

4.3.2. Upper bounds for p > 2

Theorem 4.12 gives the best possible bound on $||A||_p$ of any matrix A and any p > 2. This bound works also for graphs, but unfortunately it is never exact, for adjacency matrices have zero diagonal. Thus, the upper bounds on $||G||_p$ gives rise to some subtle problems, which are not resolved yet.

We start with the following approximate result:

Proposition 4.26. If p > 2 and G is a graph with m edges, then

$$||G||_p^p < 2m\left(-\frac{1}{2} + \sqrt{2m + \frac{1}{4}}\right)^{p-2}.$$
 (54)

The inequality is tight, since for every m, there is a graph with m edges satisfying

$$||G||_p > -\frac{3}{2} + \sqrt{2m + \frac{1}{4}}.$$
 (55)

Proof. Let p > 2 and G be a graph of order n and size m, that is to say

$$\sigma_1^2(G) + \dots + \sigma_n^2(G) = 2m. \tag{56}$$

We want to maximize $||G||_p^p$ subject to (56). First, note that

$$\sigma_1^p(G) + \dots + \sigma_n^p(G) \le \sigma_1^{p-2}(G) \left(\sigma_1^2(G) + \dots + \sigma_n^2(G)\right) = \sigma_1^{p-2}(G) 2m.$$
 (57)

On the other hand, Stanley's bound [43] implies that

$$\sigma_1(G) = \lambda_1(G) \le -\frac{1}{2} + \sqrt{2m + \frac{1}{4}},$$
(58)

and (54) follows. The inequality is strict, because if equality holds in (58), then G is a complete graph with possibly isolated vertices, and in that case inequality (57) is strict.

To see the validity of (55), consider the maximal complete graph K_s that can be formed with at most m edges. This means

$$\binom{s+1}{2} > m$$

and so

$$s > -\frac{1}{2} + \sqrt{2m + \frac{1}{4}}.$$

Hence,

$$||K_s||_p > s - 1 > -\frac{3}{2} + \sqrt{2m + \frac{1}{4}}.$$

Clearly, inequality (55) shows that (54) is asymptotically tight, for the right side of (54) satisfies

$$2m\left(-\frac{1}{2} + \sqrt{2m + \frac{1}{4}}\right)^{p-2} < (2m)^p$$
.

Proposition 4.26 is proved. \Box

Proposition 4.26 is just a tight asymptotic result and equality never holds in (54). This observation prompts the following conjecture:

Conjecture 4.27. If p > 2 and G is a graph of size m, then

$$||G||_p^p \le \left(-\frac{1}{2} + \sqrt{2m + \frac{1}{4}}\right)^p - \frac{1}{2} + \sqrt{2m + \frac{1}{4}}.$$

Equality holds if and only if G is a complete graph with possibly some isolated vertices.

Finally, we want an upper bound on $||G||_p$ in terms of the order of G. Thus, using (54), we see that if G is a graph of order n, then

$$||G||_{p}^{p} < (n-1)^{p} + (n-1)^{p-1}$$
. (59)

Since $||K||_p^p = (n-1)^p + n - 1$, bound (59) is asymptotically tight. However, equality never holds in (59), and the following conjecture is plausible:

Conjecture 4.28. If p > 2 and G is a graph of order n, then

$$\|G\|_p^p < \|K\|_p^p,$$

unless $G = K_n$.

Note that if Conjecture 4.27 is true, then Conjecture 4.28 is true as well.

4.3.3. Lower bounds

For q = 2 Corollary 4.22 gives the lower bound:

Corollary 4.29. Let p > 2. If G is a graph of order n, size m, and largest eigenvalue λ , then

$$||G||_{p}^{p} \ge \lambda^{p} + (n-1)^{1-p/2} (2m - \lambda^{2})^{p/2}.$$
 (60)

Equality holds in (60) if and only if $\sigma_2(G) = \cdots = \sigma_n(G)$.

As with all bounds of this type, Proposition 4.29 is most valuable as a device to convert lower bounds on $\lambda(G)$ into lower bounds on $\|G\|_p$; hence, following the argument after Proposition 4.24, we come up with infinitely many lower bounds on $\|G\|_p$.

In particular, we get a twin proposition of Proposition 4.24, yielding a lower bound this time:

Theorem 4.30. Let p > 2 and $m \ge n/2$. If G is a graph of order n and size m, then

$$||G||_p^p \ge (2m/n)^p + (n-1)^{1-p/2} \left(2m - (2m/n)^2\right)^{p/2}.$$
 (61)

Equality holds if and only if G is either $(n/2) K_2$, or K_n , or a design graph.

Theorem 4.30 has implications outside of the study of graph energy, e.g., the following extremal result holds:

Corollary 4.31. Let $k \geq 2$, $m \geq n/2$, and let G be a graph of order n and size m. Then the number of closed walks of length 2k of G is at least

$$\frac{1}{4k} \left((2m/n)^{2k} + (n-1)^{1-k} \left(2m - (2m/n)^2 \right)^k \right),\,$$

with equality holding if and only if G is either $(n/2) K_2$, or K_n , or a design graph.

Finally, we note a natural extension of the simple bound (15):

Corollary 4.32. If $2 > p \ge 1$ and G is a nonempty graph with m edges and largest eigenvalue λ , then

$$||G||_p^p \ge \lambda^p + \frac{2m - \lambda^2}{\sigma_2^{2-p}(G)}.$$

Equality holds if and only if all nonzero eigenvalues of G other than λ have the same absolute value.

4.4. Bounds based on Hölder's inequality

In recent years much attention has been paid to the "spectral moments method" in graph energy (see, e.g., [40,41,49,50,14]). In this section we study this topic in the light of Hölder's inequality and use Schatten norms to express the results.

Recall the classical Hölder inequality: Let $x = [x_i]$ and $y = [y_i]$ be real nonzero vectors. If the positive numbers s and t satisfy 1/s + 1/t = 1, then

$$x_1 y_1 + \dots + x_n y_n \le |[x_i]|_s |[y_i]|_t.$$
 (62)

If equality holds, then $(|x_1|^s, \ldots, |x_n|^s)$ and $(|y_1|^t, \ldots, |y_n|^t)$ are collinear. Hölder's inequality easily implies the following simple result:

Proposition 4.33. Let p > 0, q > 0, $\alpha > 0$, $\beta > 0$, and $\alpha + \beta = 1$. If a_1, \ldots, a_n are positive numbers, then

$$a_1^{\alpha p + \beta q} + \dots + a_n^{\alpha p + \beta q} \le \left(a_1^p + \dots + a_n^p\right)^{\alpha} \left(a_1^q + \dots + a_n^q\right)^{\beta}$$

If $\alpha p \neq \beta q$, then equality holds if and only if $a_1 = \cdots = a_n$.

Proof. Let $(x_1, \ldots, x_n) := (a_1^{\alpha p}, \ldots, a_n^{\alpha p})$ and $(y_1, \ldots, y_n) := (a_1^{\beta q}, \ldots, a_n^{\beta q})$. Applying (62) with $s := 1/\alpha$ and $t := 1/\beta$, we find that

$$a_1^{\alpha p + \beta q} + \dots + a_n^{\alpha p + \beta q} \le (a_1^p + \dots + a_n^p)^{\alpha} (a_1^q + \dots + a_n^q)^{\beta}.$$

If equality holds, then $(a_1^{\alpha p}, \ldots, a_n^{\alpha p})$ is collinear to $(a_1^{\beta q}, \ldots, a_n^{\beta q})$. If $\alpha p \neq \beta q$, this can happen if and only if $a_1 = \cdots = a_n$. \square

Now we get a fairly abstract inequality about the Schatten norms of arbitrary matrices:

Corollary 4.34. Let p > 0, q > 0, $\alpha > 0$, $\beta > 0$, and $\alpha + \beta = 1$. If A is a matrix, then

$$||A||_p^{\alpha p} ||A||_q^{\beta q} \ge ||A||_{\alpha p + \beta q}^{\alpha p + \beta q}$$

If $\alpha p \neq \beta q$, then equality holds if and only if all nonzero singular values of A are equal.

Slightly weaker versions of Proposition 4.33 were proved in [40] and [50]. The case $p=4, q=1, \alpha=1/3$, and $\beta=2/3$ of Proposition 4.33 was proved by Rada and Tineo in [41], and by Zhou in [49], and later rediscovered several times:

Corollary 4.35. If a_1, \ldots, a_n are nonnegative numbers, then

$$(a_1^2 + \dots + a_n^2)^3 \le (a_1 + \dots + a_n)^2 (a_1^4 + \dots + a_n^4).$$

Equality holds if and only if all nonzero numbers among a_1, \ldots, a_n are equal.

Rada and Tineo [41], and Zhou [49] also deduced the following corollary:

Corollary 4.36. Let G be a graph with m edges and q closed walks of length four. Then

$$q \|G\|_{*}^{2} \geq m^{3}$$
.

Equality holds if and only if G is a disjoint union of isolated vertices and complete bipartite graphs with the same number of edges.

Clearly, Corollary 4.34 leads to the following generalization of the above result:

Corollary 4.37. Let p > 0, q > 0, $\alpha > 0$, $\beta > 0$, and $\alpha + \beta = 1$. If A is a matrix, then

$$||G||_p^{\alpha p} ||G||_q^{\beta q} \ge ||G||_{\alpha p + \beta q}^{\alpha p + \beta q}.$$

Equality holds if and only if G is a disjoint union of isolated vertices and complete bipartite graphs with the same number of edges.

4.5. The Schatten norms of r-partite matrices and graphs

In this section we study the Schatten norms of r-partite graphs and matrices, extending some results about the trace norm obtained in [35] and presented in Section 2.3. These new extensions are published here for the first time, so we shall give full proofs.

Write $T_r(n)$ for the complete r-partite graph of order n with vertex classes of size $\lfloor n/r \rfloor$ or $\lceil n/r \rceil$, and recall that $T_r(n)$ is known as the r-partite Turán graph of order n. The number of edges $t_r(n)$ of $T_r(n)$ is well studied in connection with the Turán theorem [44]; in particular, it is known that

$$\frac{r-1}{2r}n^2 - \frac{r}{8} \le t_r(n) \le \frac{r-1}{2r}n^2.$$

4.5.1. r-Partite matrices

We start with a bound on the pivotal Schatten 2-norm $\|A\|_2$ (the Frobenius norm) of an r-partite matrix A:

Proposition 4.38. Let $n \ge r \ge 2$, and let $A = [a_{i,j}]$ be an $n \times n$ matrix with $||A||_{\max} \le 1$. If A is r-partite, then

$$||A||_2 \le \sqrt{2t_r(n)}. (63)$$

Equality holds if and only if the matrix $|A| = [|a_{i,j}|]$ is the adjacency matrix of $T_r(n)$.

Proof. Let A be an r-partite matrix satisfying the premises and let $[n] = N_1 \cup \cdots \cup N_r$ be a partition such that $A[N_i, N_i] = 0$ for any $i \in [r]$.

Define a graph G with V(G) = [n] such that i is adjacent to j whenever $|a_{i,j}| + |a_{j,i}| \neq 0$. Since the sets N_1, \ldots, N_r induce no edges in G, we see that G is r-partite. Now Turán's theorem [44] implies that

$$2e\left(G\right) < 2t_{r}\left(n\right)$$

unless $G = T_r(n)$. Hence,

$$||A||_{2}^{2} = \sum_{i,j \in [n]} |a_{i,j}|^{2} \le \sum_{i,j \in [n]} |a_{i,j}| \le \sum_{\{i,j\} \in E(G)} |a_{i,j}| + |a_{j,i}| \le 2e(G) \le 2t_{r}(n).$$

If equality holds, then $G = T_r(n)$, and $|a_{i,j}| = |a_{j,i}| = 1$ for every edge $\{i, j\} \in E(G)$. Hence |A| is the adjacency matrix of $T_r(n)$.

If |A| is the adjacency matrix of $T_r(n)$, then $||A||_2^2 = |||A|||_2^2 = 2t_r(n)$, and so A forces equality in (63). \square

Now, we easily get the following corollary:

Corollary 4.39. Let $n \ge r \ge 2$, and let $A = [a_{i,j}]$ be an $n \times n$ matrix with $||A||_{\max} \le 1$. If A is r-partite, then

$$\|A\|_2 \le n\sqrt{1 - 1/r}.$$

If $[n] = N_1 \cup \cdots \cup N_r$ is a partition such that $A[N_i, N_i] = 0$ for any $i \in [r]$, then equality holds if and only if $|N_1| = \cdots = |N_r|$, and $|a_{i,j}| = 1$ whenever i and j do not belong to the same partition set.

Armed with Corollary 4.39, we are ready to give an upper bound on the Schatten p-norm of a complex r-partite matrix whenever $2 > p \ge 1$.

Theorem 4.40. Let $n \ge r \ge 2$, $2 > p \ge 1$, and let $A = [a_{i,j}]$ be an $n \times n$ matrix with $||A||_{\max} \le 1$. If A is r-partite, then

$$||A||_p \le n^{1/2+1/p} \sqrt{1-1/r}.$$

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

Proof. Let A be an r-partite matrix satisfying the premises, and suppose that $[n] = N_1 \cup \cdots \cup N_r$ is a partition such that $A[N_i, N_i] = 0$ for any $i \in [r]$. Let $\sigma_1, \ldots, \sigma_n$ be the singular values of A. Our starting point is Proposition 4.38, which gives

$$\sigma_1^2 + \dots + \sigma_n^2 = \sum_{i,j \in [n]} |a_{i,j}|^2 \le \left(1 - \frac{1}{r}\right) n^2.$$

This bound and the PM inequality imply that

$$\left(\frac{\sigma_1^p + \dots + \sigma_n^p}{n}\right)^{1/p} \le \left(\frac{\sigma_1^2 + \dots + \sigma_n^2}{n}\right)^{1/2} \le (1 - 1/r)^{1/2} n^{1/2}.$$
(64)

Hence,

$$||A||_p = \left(\frac{\sigma_1^p + \dots + \sigma_n^p}{n}\right)^{1/p} \le n^{1/2 + 1/p} \sqrt{1 - 1/r},$$

as stated.

If $||A||_p = n^{1/2+1/p} \sqrt{1-1/r}$, then the condition for equality in the PM inequality used in (64) implies that

$$\sigma_1 = \dots = \sigma_n = \sqrt{(1 - 1/r) n},$$

completing the proof. \Box

Next, we show that if r is the order of a conference matrix, then bound (16) in Theorem 4.40 is best possible for infinitely many n.

Theorem 4.41. Let r be the order of a conference matrix, and let k be the order of an Hadamard matrix. If $p \geq 1$, there exists an r-partite matrix A of order n = rk with $\|A\|_{\max} = 1$ such that

$$||A||_p = n^{1/2 + 1/p} \sqrt{1 - 1/r}.$$

Proof. Let C be a conference matrix of order r and H be an Hadamard matrix of order k. First, note that

$$||C||_p = \left(r\left(\sqrt{r-1}\right)^p\right)^{1/p} = r^{1/p}\sqrt{r-1},$$

and

$$||H||_p = \left(k\left(\sqrt{k}\right)^p\right)^{1/p} = k^{1/p+1/2}.$$

Next, 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 that $A[N_i, N_i] = 0$ for any $i \in [r]$.

Finally, we find that

$$\begin{split} \|A\|_p &= \|C \otimes H\|_p = \|C\|_p \, \|H\|_p \\ &= k^{1/p+1/2} r^{1/p} \sqrt{r-1} = (kr)^{1/2+1/p} \, \sqrt{1-1/r} \\ &= n^{1/2+1/p} \sqrt{1-1/r}, \end{split}$$

completing the proof of Theorem 4.41. \Box

We have no results about the Schatten p-norms of r-partite matrices for p > 2. The reader may be interested in the following conjecture:

Conjecture 4.42. Let p > 2, $n \ge r \ge 2$, and let $A = [a_{i,j}]$ be an $n \times n$ complex matrix with $||A||_{\max} \le 1$. If A is r-partite, then

$$||A||_p \leq ||T_r(n)||_p.$$

Equality holds if and only if the matrix $|A| = [|a_{i,j}|]$ is the adjacency matrix of $T_r(n)$.

4.5.2. r-Partite graphs

Similarly to Problem 2.14, we raise the following natural problem about graphs:

Problem 4.43. What is the maximum Schatten *p*-norm of an *r*-partite graph of order *n*?

Our starting point is Theorem 4.40, which implies a bound for nonnegative matrices, in particular, for graphs.

To simplify the subsequent proofs, first we give a uniform bound on the Schatten p-norm of a complete multipartite graph.

Proposition 4.44. If $p \ge 1$ and K is a complete r-partite graph of order n, then

$$||K||_{p} \le 2(1-1/r)n.$$
 (65)

Proof. Indeed, Propositions 4.2 and 4.3 imply that $||K||_p \leq ||K||_*$, and the result of Caporossi, Cvetković, Gutman, and Hansen [6] implies that $||K||_* = 2\lambda_1(K)$. Finally, recall that Cvetković [8] showed that $\lambda_1(K) \leq (1 - 1/r) n$, completing the proof. \square

Note that bound (65) is best possible for p = 1, and is within a factor of 2 of the best possible for any p > 1. Indeed, if K is a complete regular r-partite graph, then

$$||K||_p > \lambda_1(K) = (1 - 1/r) n.$$

Theorem 4.45. Let $n \ge r \ge 2$, $2 > p \ge 1$, and let A be an $n \times n$ nonnegative matrix with $||A||_{\max} \le 1$. If A is r-partite, then

$$||A||_p \le \frac{1}{2} n^{1/2 + 1/p} \sqrt{1 - 1/r} + (1 - 1/r) n.$$

Proof. Let A be an r-partite matrix satisfying the premises, and suppose that $[n] = N_1 \cup \cdots \cup N_r$ is a partition such that $A[N_i, N_i] = 0$ for any $i \in [r]$.

For each $i \in [r]$, set $n_i := |N_i|$, and write K for the matrix obtained from J_n by zeroing the submatrices $J_n[N_i, N_i]$ for each $i \in [r]$. Note that K is the adjacency matrix of the complete r-partite graph with vertex classes N_1, \ldots, N_r .

Now, let B := 2A - K, and note that the matrix B and the sets N_1, \ldots, N_r satisfy the premises of Theorem 4.40; hence the triangle inequality implies that

$$\begin{split} n^{1/2+1/p} \sqrt{1-1/r} &\geq \|B\|_p \geq \|2A-K\|_p \\ &\geq 2 \, \|A\|_p - \|K\|_p \geq 2 \, \|A\|_p - 2 \, (1-1/r) \, n, \end{split}$$

completing the proof of Theorem 2.20. \Box

Note that the matrix A in Theorems 4.40 and 4.45 needs not be symmetric; nonetheless, the following immediate corollary is tight up to an additive term that is linear in n:

Corollary 4.46. Let $n \ge r \ge 2$ and $2 > p \ge 1$. If G is an r-partite graph of order n, then

$$||G||_p \le \frac{1}{2} n^{1/2 + 1/p} \sqrt{1 - 1/r} + (1 - 1/r) n.$$
 (66)

To prove the tightness of Theorems 4.45 and Corollary 4.46, we modify the construction in Theorem 4.41 as follows:

Theorem 4.47. Let $2 > p \ge 1$ and 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 such that

$$||G||_p \ge \frac{1}{2} n^{1/2 + 1/p} \sqrt{1 - 1/r} - (1 - 1/r) n.$$

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 that $B[N_i, N_j]$ is a (-1, 1)-matrix for any $i, j \in [r]$ with $i \neq j$. Finally, set $K_t := J_t - I_t$ and let

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

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.

Next, note that the singular values of B are equal to

$$\sqrt{k(r-1)} = \sqrt{(1-1/r) n}.$$

Thus, the triangle inequality implies that

$$\|(B + K_r \otimes J_k)\|_p \ge \|B\|_p - \|K_r \otimes J_k\|_p \ge n^{1/2 + 1/p} \sqrt{1 - 1/r} - 2(1 - 1/r)n,$$

and so,

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

completing the proof of Theorem 4.47. \Box

Concrete examples of the above construction can be found using, e.g., Paley's conference and Hadamard matrices described in Section 2.3.

If p=2, let us note the following simple result of extremal graph theory:

If $n \geq r$ and G is an r-partite graph of order n, then $||G||_2 < ||T_r(n)||_2$, unless $G = T_r(n)$.

However, it is not so easy to generalize this statement for p > 2. The following conjecture seems plausible:

Conjecture 4.48. If p > 2, $n \ge r$, and G is an r-partite graph of order n, then

$$\left\|G\right\|_{p} < \left\|T_{r}\left(n\right)\right\|_{p},$$

unless $G = T_r(n)$.

4.6. The Schatten norms of trees

In [7], Csikvári showed that the path has the minimum number of closed walks of any given length among all connected graphs of given order, and the star has the maximum number of closed walks of any given length among all trees of given order.

These results can be expressed in Schatten norms as follows:

Proposition 4.49. If G is a connected graph of order n, then $||G||_{2k} \ge ||P_n||_{2k}$ for every integer $k \ge 2$.

Proposition 4.50. If T is a tree of order n, then $||T||_{2k} \leq ||S_n||_{2k}$ for every integer $k \geq 2$.

On the other hand, it is known that the path has maximal energy among all trees of given order and the star has minimal energy among all connected graphs of given order. These facts lead us to the following natural questions:

Question 4.51. Let G be a connected graph of order n.

- (a) Is it true that $||G||_p \ge ||P_n||_p$ for every p > 2?
- (b) Is it true that $||G||_p \ge ||S_n||_p$ for every 1 ?

Question 4.52. Let T be a tree of order n.

(a) Is it true that

$$||S_n||_n \ge ||T||_n \ge ||P_n||_n$$

for every p > 2?

(b) Is it true that

$$||P_n||_p \ge ||T||_p \ge ||S_n||_p$$

for every 1 ?

Let us note that the techniques that work for the norm $||G||_{2k}$ for integer k are not directly applicable to the above questions.

4.7. The Schatten norms of almost all graphs

Our last topic provides some insight into the Schatten p-norm of the "average" graph of order n. In [34], the following theorem was proved:

Theorem 4.53. If G is a graph of order n, then with probability tending to 1:

(i) if $2 > p \ge 1$, then

$$||G||_{p} = \left(\frac{1}{\sqrt{\pi}} \cdot \frac{\Gamma(p/2 + 1/2)}{\Gamma(p/2 + 2)} + o(1)\right)^{1/p} n^{1/p + 1/2}; \tag{67}$$

(ii) if p = 2, then

$$\left\|G\right\|_{p} = \left(1/\sqrt{2} + o\left(1\right)\right)n;$$

(iii) if p > 2, then

$$||G||_p = (1/2 + o(1)) n.$$

The proof is based on the assumption that the spectrum of the "average graph" of order n is approximated by the spectrum of the Erdős–Rényi random graph G(n, 1/2). Recall that in G(n, 1/2) every pair of vertices is joined independently with probability 1/2.

If p > 2, the value of $||G||_p$ is determined essentially by the largest eigenvalue of G, which is almost surely n/2 + o(n). This implies (iii).

If p = 2, then $||G||_2^2$ is equal to twice the number of edges of G, which is almost surely $(1/2 + o(1)) n^2$, implying (ii).

Finally, for $2 > p \ge 1$, one can use Wigner's semicircle law and calculate the required value, getting (i).

The three cases $2 > p \ge 1$, p = 2, and p > 2 are quite disparate and seem to contradict Proposition 4.1, which claims that $||G||_p$ is differentiable in p for $p \ge 1$. However, in Theorem 4.53 it is supposed that p is fixed and $n \to \infty$. Thus, the three instances of the term o(1) depend on p and are different in each case.

Let us note that calculating the right side of (67) for p = 1, we see that the energy of almost all graphs of order n is almost surely equal to

$$\left(\frac{4}{3\pi} + o(1)\right)n^{3/2}.$$

This basic fact has been established in [31].

4.7.1. Concluding remark

We hope to have shown that matrix norms of graphs are a vital and challenging topic, which throws bridges between analysis and combinatorics. Also, we hope to have shown that the core research on graph energy has strong ties to mainstream mathematics. Let us hope that by exploring and expanding these connections, future research on graph energy shall keep flourishing.

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