Graphs with Integral Spectrum

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Abstract

It is shown that only a fraction of $2^{-\Omega(n)}$ of the graphs on n vertices have an integral spectrum. Although there are several explicit constructions of such graphs, no upper bound for their number has been known. Graphs of this type play an important role in quantum networks supporting the so-called perfect state transfer.

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1 Introduction

We say that a graph is integral if all the eigenvalues of its adjacency matrix are integers. The notion of integral graphs dates back to F. Harary and A. J. Schwenk [15]. Furthermore, several explicit constructions of integral graphs of special types appear in the literature, see [3, 4, 5, 6, 16, 17, 21, 22, 27, 28] and references therein.

It has recently been discovered that integral graphs may be of interest for designing the network topology of perfect state transfer networks, see [1, 8, 7, 12, 14, 20].

However it seems that no nontrivial upper bounds on the total number of integral graphs with n vertices have been known. It is natural to expect that this number is negligible compared to the total number of graphs. Here we obtain an estimate which shows that this is the case, although we believe our bound is far from being tight and the number of integral graphs is substantially smaller.

In fact it is easier to work in terms of adjacency matrices. Namely, let $\mathcal{A}_n$ be the set of all adjacency matrices of graphs with n vertices. That is, $\mathcal{A}_n$ is the set of symmetric $0,1$-matrices $A = (a_{ij})_{i,j=1}^n$ of dimension n with zeros on the main diagonal,

$$a_{ij} = a_{ji} \in \{0, 1\}, \quad a_{ii} = 0, \qquad i, j = 1, \ldots, n.$$

Accordingly we denote by $I(n)$ the total number of adjacency matrices $A \in \mathcal{A}_n$ such that all eigenvalues of A are integer numbers.

We note that despite a recent series of very strong results [2, 9, 23, 24, 25, 26] treating various counting questions for $0,1$-matrices, no upper bounds on $I(n)$ have been known prior to our work, which derives the following result:

Theorem 1. *For a sufficiently large n, We have*

$$I(n) \leq 2^{n(n-1)/2-n/400}.$$

Note that the first part of the expression, $2^{n(n-1)/2}$, is the number of graphs on n vertices.

2 Distribution of Eigenvalues

We remark that if A is chosen uniformly at random from $\mathcal{A}_n$ then it can be described as an n-dimensional random symmetric $0,1$-matrix whose entries for $1 \leq i < j \leq n$ are independent random variables taking values 0 and 1 with probability $1/2$ and also $a_{ii} = 0$ with probability 1 for $1 \leq i \leq n$.

Thus random matrices from $\mathcal{A}_n$ fit in the models used by [2, 13] which provide our main tools.

As A is symmetric its eigenvalues are real and we denote them by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

We start with the following result on the distribution of eigenvalues of random matrices, which is due to Z. Füredi and J. Komlós [13].

Lemma 2. *Let A be chosen uniformly at random from $\mathcal{A}_n$. Then for any $c > 1$ and for all the eigenvalues λ_i, $i = 2, \ldots, n$ of A but the largest one λ_1, with probability at least $1 - n^{-10}$ we have*

$$-c\sqrt{n} < \lambda_i < c\sqrt{n}, \qquad i = 2, \ldots, n,$$

for large enough values of n.

Furthermore let E_i denote the expected value of the i-th largest eigenvalue λ_i of A. Then Lemma 2 leads to the following estimate on E_i.

Corollary 3. *Let A be chosen uniformly at random from $\mathcal{A}_n$. Then*

$$|E_i| < 2\sqrt{n}$$

for $i > 1$ and large enough values of n.

Proof. Notice that if λ is an eigenvalue of A, then $-n < \lambda < n$. Now using Lemma 2 with $c = 3/2$, we have that with probability $1 - n^{-10}$, λ_i for $i > 1$ is at most $3\sqrt{n}/2$ and with probability n^{-10} it is at most n. Thus

$$E_i < \left(1 - \frac{1}{n^{10}}\right)\frac{3}{2}\sqrt{n} + \frac{1}{n^{10}}n < 2\sqrt{n}$$

for large enough values of n. Similarly we have

$$E_i > \left(1 - \frac{1}{n^{10}}\right)\frac{-3}{2}\sqrt{n} + \frac{1}{n^{10}}(-n) > -2\sqrt{n},$$

which concludes the proof. $\square$

Let M_i denote the median of the i-th largest eigenvalue λ_i of $A \in \mathcal{A}_n$. That is M_i is the smallest real such that for at least $0.5\#\mathcal{A}_n$ matrices $A \in \mathcal{A}_n$ we have $\lambda_i \geq M_i$.

Corollary 4. *We have*

$$|M_i| < 6\sqrt{n}, \qquad i = 2, \ldots, n.$$

Proof. Suppose that $M_i \geq 6\sqrt{n}$. Then using Lemma 2 with $c = 3/2$ we obtain

$$E_i \geq \frac{1}{2}(6\sqrt{n}) + \frac{1}{2}\left(\frac{-3}{2}\sqrt{n}\right) + \frac{1}{n^{10}}(-n) \geq 2\sqrt{n}.$$

which contradicts Corollary 3. Similarly $M_i > -6\sqrt{n}$. $\square$

The following result from [2] is also crucial for what follows.

Lemma 5. *Let A be chosen uniformly at random from $\mathcal{A}_n$. Then*

$$\Pr_{A\in\mathcal{A}_n}\left[|\lambda_s - M_s| > t\right] \leq 4e^{-t^2/8r^2}$$

where $r = \min\{s, n-s+1\}$.

From Corollary 4 and Lemma 5 we derive:

Corollary 6. *Let A be chosen uniformly at random from $\mathcal{A}_n$ and λ be any eigenvalue of A but the largest one. Then with probability at least $1 - 8e^{-n/32}$ we have*

$$-7\sqrt{n} < \lambda < 7\sqrt{n}.$$

Proof. Using Corollary 4 we have

$$\Pr_{A\in\mathcal{A}_n}\left[\lambda_2 > 7\sqrt{n}\right] = \Pr_{A\in\mathcal{A}_n}\left[\lambda_2 - 6\sqrt{n} > \sqrt{n}\right] \le \Pr_{A\in\mathcal{A}_n}\left[\lambda_2 - M_2 > \sqrt{n}\right].$$

Now applying Lemma 5 with $t = \sqrt{n}$ we have

$$\Pr_{A\in\mathcal{A}_n}\left[\lambda_2 > 7\sqrt{n}\right] \le 4e^{-n/32}.$$

Similarly we have

$$\Pr_{A\in\mathcal{A}_n}\left[\lambda_n < -7\sqrt{n}\right] \le 4e^{-n/32}.$$

Now assume that P is the probability that all the eigenvalues but the largest one are between $-7\sqrt{n}$ and $7\sqrt{n}$. Then

$$P \ge 1 - \Pr_{A\in\mathcal{A}_n}\left[\lambda_n < -7\sqrt{n}\right] - \Pr_{A\in\mathcal{A}_n}\left[\lambda_2 > 7\sqrt{n}\right] \ge 1 - 8e^{-n/32},$$

which concludes the proof. □

3 Multiplicities of Eigenvalues

Let M be a square matrix of order n. Then a principal submatrix of order r of M is a submatrix of M obtained by deleting rows $R_{i_1}, R_{i_2}, \ldots, R_{i_{n-r}}$ and columns $C_{i_1}, C_{i_2}, \ldots, C_{i_{n-r}}$ where $1 \le i_1 \le i_2 \le \ldots \le i_{n-r} \le n$. Notice that all the principal submatrices of a symmetric matrix are symmetric too.

We recall that if λ is an eigenvalue of the matrix M, then its algebraic multiplicity is its order as a root of the characteristic polynomial of M and its geometric multiplicity is the rank of the null-space of $M - \lambda I$. We also recall that if λ is an eigenvalue of a symmetric matrix M, then the algebraic multiplicity of λ is equal to its geometric multiplicity.

The following result, (see, for example, [19, Theorem 5.19] and many other standard linear algebra books about the principal sub-matrices of symmetric matrices) is a consequence of the expansion of the coefficients of the characteristic polynomial in terms of minors and the fact that eigenvalues of symmetric matrices have the same algebraic and geometric multiplicity.

Lemma 7. *Let M be a symmetric matrix. Then M is of rank r if and only if M has a nonsingular principal submatrix of order r and has no larger principal submatrix which is nonsingular.*

Our next results can be of independent interest.

Lemma 8. *Let λ be an eigenvalue of algebraic multiplicity s of an adjacency matrix of order n. Then $|\lambda| + s \leq n$.*

Proof. Let A be an adjacency matrix having λ as an eigenvalue of algebraic multiplicity s. Since A is a symmetric matrix, λ is of geometric multiplicity s meaning that the rank of $A_\lambda = A - \lambda I$ is $n - s$. Now (the easy part of) Lemma 7 implies that all the principal submatrices of order $n - s + 1$ of A_λ are singular. This in turn means that λ is an eigenvalue of all the principal submatrices of order $n - s + 1$ of A. But all the principal submatrices of A are adjacency matrices of some graphs, and thus the absolute value of their eigenvalues is bounded above by their order minus one. Hence $|\lambda| \leq (n - s + 1) - 1 = n - s$. This completes the proof. $\square$

Lemma 9. *Let λ be a real number. Then the number $N_\lambda(n, s)$ of adjacency matrices of order n having λ as an eigenvalue of algebraic multiplicity s is at most*

$$N_\lambda(n, s) \leq \binom{n}{s} 2^{n(n-1)/2 - s(s-1)/2}.$$

Proof. Let A be an adjacency matrix having λ as an eigenvalue of algebraic multiplicity s. Since A is a symmetric matrix, λ is of geometric multiplicity s meaning that the rank of $A_\lambda = A - \lambda I$ is $n - s$. Now Lemma 7 implies that there is a principal submatrix B of order $n - s$ of A_λ which is nonsingular. Suppose that B corresponds to rows $R_{i_1}, R_{i_2}, \ldots, R_{i_{n-s}}$ and columns $C_{i_1}, C_{i_2}, \ldots, C_{i_{n-s}}$ of A_λ. Notice that $C_{i_j}^T = R_{i_j}$. We claim that the entries at rows $R_{i_1}, R_{i_2}, \ldots, R_{i_{n-s}}$ and columns $C_{i_1}, C_{i_2}, \ldots, C_{i_{n-s}}$ of A_λ uniquely determines the rest of the entries of A_λ and hence determine A.

To prove this claim, let C be the $(n-s) \times n$ submatrix of A_λ consisting of $R_{i_1}, R_{i_2}, \ldots, R_{i_{n-s}}$ and let D be the $n \times (n-s)$ submatrix of A_λ consisting of $C_{i_1}, C_{i_2}, \ldots, C_{i_{n-s}}$. Notice that B is a submatrix of both matrices C and D. Since B is a nonsingular matrix of order $n-s$ and C is an $(n-s) \times n$ matrix, it follows that the columns of B span the columns of C. This means that every column of C is a unique linear combination of columns of B which in turn means that every column of A_λ is a unique linear combination of columns of D. Thus given all the entries of C and D uniquely determines the rest of the entries of A_λ and hence A. $\square$

4 Concluding the Proof of Theorem 1

By Corollary 6 the number of matrices which have at least one more eigenvalue other than the largest one either greater than $7\sqrt{n}$ or less than $-7\sqrt{n}$ is at most $8e^{-n/32}2^{n(n-1)/2}$ and all the eigenvalues but the largest one of the remaining matrices are bounded by $-7\sqrt{n}$ and $7\sqrt{n}$. This means that a matrix in the latter case having integral spectrum should have one eigenvalue of algebraic and geometric multiplicity at least

$$t = \frac{n-1}{14\sqrt{n}+1}.$$

Thus, using Lemmas 9 and 8 we see that there are at most

$$\sum_{-7\sqrt{n}\le\lambda\le 7\sqrt{n}} \sum_{t\le s\le n-|\lambda|} N_\lambda(n,s) \le (14\sqrt{n}+1)\binom{n}{t} 2^{n(n-1)/2-t(t-1)/2+1}$$

matrices in this set having an integral spectrum. This completes the proof.

□

5 Remarks and Further Questions

The results of [2, 13] hold for more general sets of matrices than adjacency matrices. Accordingly, the ideas of this paper can be used to obtain analogues of our results in more general settings.

Note that by [21, Corollary 7.2] there are at most $2^{\tau(n)-1}$ integral circulant graphs on n vertices, where $\tau(n)$ is the number of positive integer divisors of n.

The results of this work appear to be rather weak and a stronger bound would be of interest. The problem seems somewhat related to the problem of determining which graphs are determined by their spectra (referred to as DS graphs in [11]). It is commented there that while the fraction of known non-DS graphs on n-vertices is much larger than the fraction of known DS graphs, both fractions (of known graphs of these types) tend to zero as $n \to \infty$. E. van Dam and W. Haemers [11] state:

> If we were to bet, it would be for: 'almost all graphs are DS'.

As the total number of ways of choosing a multiset of n integers in the interval $[-(n-1),(n-1)]$ is only $2^{O(n)}$, a good upper estimate for the number of graphs with the same spectrum may provide a tight upper bound for our problem as well. Similarly, the number of possible integral spectra of r-regular graphs on n vertices is only $n^{O(r)}$, showing that a good upper bound for the number of r-regular integral graphs would follow from an effective upper estimate on the maximum possible number of cospectral r-regular graphs on n vertices.

Unfortunately this approach does not seem fruitful at the moment, as it leads to a problem that does not appear to be easier than the original question.

A lower bound on the number of (isomorphism classes of) integral graphs with n vertices is at least $2^{\Omega(n)}$. This follows for $n = 2^k$ from the fact that any Cayley Graph of $(\mathbb{Z}_2)^k$ is integral. Similarly, for $n = 4^k$, any Cayley graph of $(\mathbb{Z}_4)^k$ is integral. Indeed, the eigenvalues of Cayley graphs of abelian groups are sums of characters of the group (c.f., for example, [18]), showing that in the first case these are sums of members of $\{\pm 1\}$ and in the second case sums of members of $\{\pm 1, \pm i\}$, which, being real numbers, are necessarily integers. For general values of n it suffices to take disjoint unions of graphs as above.

In a sense the problem addressed here is part of a much larger problem of relating eigenvalues of graphs to graph properties, a problem that has attracted considerable attention in the literature and one that has resisted significant progress, apart from the extensive work on the relation between the expansion properties of graphs and the size of their second largest eigenvalue.

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