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PARTIAL SUM OF EIGENVALUES OF RANDOM GRAPHS

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Abstract. Let G be a graph on n vertices and let $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$ be the eigenvalues of its adjacency matrix. For random graphs we investigate the sum of eigenvalues $s_k = \sum_{i=1}^{k} \lambda_i$, for $1 \leqslant k \leqslant n$, and show that a typical graph has $s_k \leqslant (e(G) + k^2)/(0.99n)^{1/2}$, where $e(G)$ is the number of edges of G. We also show bounds for the sum of eigenvalues within a given range in terms of the number of edges. The approach for the proofs was first used in Rocha (2020) to bound the partial sum of eigenvalues of the Laplacian matrix.

Keywords: sum of eigenvalues; graph energy; random matrix

MSC 2020: 05C50, 15A18

1. Introduction

Consider a graph $G = (E, V)$ on n vertices and let A be its adjacency matrix with eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$. For an undirected graph the adjacency matrix is symmetric and therefore all its eigenvalues are real. Here the partial sum $s_k(G) = \sum_{i=1}^{k} \lambda_i$, for $1 \leqslant k \leqslant n$ is investigated. The most notorious application of spectral graph theory in chemistry makes a correspondence between graph eigenvalues and the molecular orbital energy levels of π-electrons in conjugate hydrocarbons, which gives rise to the concept of graph energy. From that, understanding the behavior of s_k is of interest in theoretical chemistry in the Hückel molecular orbital (HMO) theory. Here we show upper bounds on s_k for random graphs in terms of the number of edges.

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In book [5] the main results on graph energy are surveyed. The references presented there demonstrate the long-lasting effort to understand these parameters, which as a consequence has created a great number of papers in the literature.

The method we use relies on the rich theory of random matrices. Random matrices were introduced by Eugene Wigner in [11] to model the nuclei of heavy atoms. He suggested that the gap between the lines in the spectrum of a heavy atom nucleus looks like the gap between the eigenvalues of a random matrix.

Next, we briefly describe the connection between the parameter s_k and chemistry.

1.1. Origins and applications. In HMO the behavior of the so-called π-electrons in an unsaturated conjugated molecule is described. Generally speaking, if the carbon-atom skeleton of the underlying conjugated molecule is represented as a graph, then each eigenvalue of the adjacency matrix determines the energy level of a π-electron, and the sum s_k determines the energy of electrons with the highest level of energy. Additionally, the corresponding eigenvector describes how the π-electron moves within the molecule, i.e. the molecular orbital.

Furthermore, in theoretical chemistry the sum $s_k(G)$ is of interest for certain large values of k, one in particular is $k = \lfloor \frac{n}{2} \rfloor$. However, there are some difficulties in working with $s_{\lfloor \frac{n}{2} \rfloor}(G)$ analytically. In order to approximate the quantity $s_{\lfloor \frac{n}{2} \rfloor}(G)$, in 1978 Ivan Gutman introduced the concept of energy of a graph

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

The energy relates to s_k by $E(G) = 2 \max\limits_{1 \leqslant k \leqslant n} s_k(G)$. Furthermore, for a bipartite graph we have $E(G) = 2s_{\lfloor \frac{n}{2} \rfloor}(G)$. Since its introduction, the energy of a graph has been intensively investigated. For a survey and bounds on the energy see [5], [9] and [1], [6] for further bounds on s_k.

Definitely not all graphs represent molecules, but when they do, the notion of graph energy $E(G)$ is closely related to the total π-electron energy, denoted by E_π. To be more precise, if the graph in question represents a molecule, we have $E_\pi = 2\sum\limits_{i=1}^{n/2} \lambda_i$ whenever n is even, and $E_\pi = 2 \sum\limits_{i=1}^{(n-1)/2} \lambda_i + \lambda_{(n+1)/2}$ otherwise. On a first thought, graph energy is more appealing, since mathematically it is easier to work with $E(G)$ instead of E_π, as evidenced by the number of mathematical results obtained for graph energy in contrast to total π-electron energy. However, a better reason to work with graph energy instead is the fact that $E_\pi = E(G)$, except for certain non-bipartite graphs which are irrelevant for chemical applications. (See [3] for more details.)

Before we present new bounds for s_k of random graphs, let us first mention some relevant work.

1.2. Related results. In [6] the first relevant result for our investigation is given. In that paper, Mohar showed the upper bound

$$s_k(G) \leqslant \frac{1}{2}(1+\sqrt{k})n \tag{1.1}$$

for all $1 \leqslant k \leqslant n$. He also showed that for every k there exist graphs whose sum $s_k(G)$ is $\frac{1}{2}(1+\sqrt{k})n - o(k^{-2/5})n$.

Later, in an elucidating series of papers, Nikiforov expanded the study of graph energy by looking to Ky Fan, Schatten, and trace norms of matrices. In [7], where this was first observed, the energy of matrices is introduced and the Wigner's semicircle law was applied to find hyperenergetic graphs. To that end, it was shown that for almost all graphs

$$E(G) = \Big(\frac{4}{3\pi} + o(1)\Big)n^{3/2}. \tag{1.2}$$

The claim that a property holds for almost all graphs is made precise in Section 2. Further, in [8] Nikiforov showed that several bounds such as (1.1), which were proved for graphs, can be proven in a more general setting of matrices. For a matrix A of order $m \times n$ the k-Ky Fan norm is defined by $\|A\|_{F_k} = \sum\limits_{i=1}^{k} \sigma_i$, where $\sigma_1 \geqslant \sigma_2 \geqslant \ldots \geqslant \sigma_n$ are the singular values of A. Nikiforov proved that for a matrix with entries in $[0,1]$ we have

$$\|A\|_{F_k} \leqslant \frac{1}{2}(1+\sqrt{k})\sqrt{mn} \tag{1.3}$$

for all $1 \leqslant k \leqslant n$. Notice that $s_k(G) \leqslant \|A_G\|_{F_k}$, where A_G is the adjacency matrix of a graph G, thus (1.1) follows from (1.3). We notice that if we denote by t the number of positive eigenvalues, then as a function of k, the sum s_k is increasing until t and after that it is nonincreasing, in particular $s_n = 0$, since the trace of A is zero. We recall that a regular graph is a graph where each vertex has the same degree, and therefore its adjacency matrix has the same number of ones in each row and column. In [9], Nikiforov characterizes the cases of equality when A is the adjacency matrix of a graph, which is given by certain regular graphs (see Theorem 3.6 from [9] for details). Let us say that we want to know for a fixed $k = k_0$ among all graphs with n vertices, what the extremal graphs giving equality in (1.3) look like. According to that result, for a fixed $k = k_0$ the extremal graphs that give equality in (1.3) are regular graphs where each of them has the same number of edges, say E_0. That is,

as the starting point of our investigation, instead of asking for the extreme bound for a fixed k, we want to improve the bound for a fixed number of edges.

That is a natural question. We ask for a bound on s_k among graphs with E_0 edges. By Nikiforov's characterization, the upper bound (1.3) is not tight among the graphs with E_0 edges, unless $k = k_0$. Alternatively, we can choose $k \neq k_0$ and ask for a bound on s_k among all graphs with E_0 egdes. Certainly (1.3) is not the best possible. Therefore, we have space for improvement, which is exactly the subject of our investigation. Our results reveal the order of this bound in terms of the number of edges for a typical graph.

2. New bounds

We consider the Erdős-Rényi random graph with probability p and distribution $\mathbb{G}(n,p)$, i.e., a graph drawn from this distribution has n vertices, where each pair of vertices has an edge with probability p and no edge with probability $1-p$. It is a basic fact that any graph with n vertices is equally likely in the distribution $\mathbb{G}(n,\frac{1}{2})$. Thus, we say that a property holds for almost all graphs if the probability, that a graph drawn from $\mathbb{G}(n,\frac{1}{2})$ has this property, tends to 1 as n grows. Here we will run our proofs for $\mathbb{G}(n,p)$, where $p \in (0,1)$ is a constant. However, a more careful and detailed investigation can be performed to show that the same bound holds, for example, for graphs sampled from $\mathbb{G}(n,1/n^{1-o(n)})$. From that it follows that the result holds for typical graphs where the number of edges is not necessarily around n^2.

Before we provide an explicit upper bound on s_k we would like to briefly mention how we can find such bounds and how to prove it. The approach we use here was first used by the author in [10] to bound the partial sum of eigenvalues of the Laplacian matrix. In that case, an expression for this upper bound was known in the form of a conjecture. For the adjacency matrix, we do not have such expressions a priori. However, our approach forces a bound to appear and we roughly describe this idea. Such expression arises if we can find functions f, g, and h depending on n satisfying:

(1) $\mathbb{P}[g \leqslant h(e(G_n))] \to 1$ as $n \to \infty$, where h depends on the number of edges;
(2) $\mathbb{P}[s_k(G) \leqslant f] \to 1$ as $n \to \infty$;
(3) there exists n_0 such that $f(n) \leqslant g(n)$ for $n \geqslant n_0$.

Once we find these functions, by Bonferroni's inequality we clearly have

$$\mathbb{P}[s_k(G) \leqslant h(e(G_n))] \geqslant \mathbb{P}[s_k(G) \leqslant f] + \mathbb{P}[g \leqslant h(e(G_n))] - 1 \to 1.$$

Therefore, the function h in (1) is the desired upper bound for s_k.

In the next result we explicitly describe such function. The hard part, which is to find the functions with the above properties, is described in the next proof and it relies on the limiting behavior of the eigenvalues of random graphs together with a simple concentration of the number of edges around its expectation.

Theorem 2.1. *For almost all graphs we have* $s_k(G) \leqslant (e(G) + k^2)/(0.99n)^{1/2}$.

P r o o f. To make the calculations more transparent we fix $p = \frac{1}{2}$ and notice that our proof still holds by a simple change in the constants. It was proved in [2] that the largest eigenvalue of $G(n, \frac{1}{2})$ is almost surely close to $\frac{1}{2}n$ and that the other eigenvalues almost surely have absolute values at most $\sqrt{n} + O(n^{1/3}\log n)$. For $G \sim G(n, \frac{1}{2})$ that implies

$$\mathbb{P}\Big[s_k(G) \leqslant (\sqrt{n} + O(n^{1/3}\log n))(k-1) + \frac{n}{2}\Big] \to 1. \tag{2.1}$$

Also, for any $\delta > 0$, by the Hoeffding inequality [4], we have

$$\mathbb{P}\Big(\frac{1-\delta}{2}\binom{n}{2} \leqslant e(G)\Big) \to 1 \tag{2.2}$$

as n tends to infinity.

Claim 1. There exists $\delta > 0$ such that for n large enough we have

$$(0.99n)^{1/2}\Big((\sqrt{n} + O(n^{1/3}\log n))(k-1) + \frac{n}{2}\Big) < \frac{1-\delta}{2}\binom{n}{2} + k^2. \tag{2.3}$$

P r o o f. We define a polynomial in the variable k as

$$\begin{aligned} f(k) &:= \frac{1-\delta}{2}\binom{n}{2} + k^2 - (0.99n)^{1/2}\Big((\sqrt{n} + O(n^{1/3}\log n))(k-1) + \frac{n}{2}\Big) \\ &= k^2 - k(0.99^{1/2}n + O(n^{5/6}\log n)) + \frac{1-\delta}{2}\binom{n}{2} + o(n^2). \end{aligned}$$

The discriminant of f can be written as

$$\Delta = \frac{1}{2}(0.99n^2 - (1-\delta)(n-1)n + o(n^2)).$$

Notice that we can find $N \geqslant 1$ such that for $n \geqslant N$ we have $0.991n^2 \leqslant (n-1)n$. That implies

$$2\Delta \leqslant (-0.001 + 0.991\delta)n^2 + o(n^2).$$

Now, by fixing $\delta < \frac{0.001}{0.991}$ we obtain $\Delta < 0$ for n large enough, which implies $f(k) > 0$ and (2.3) for n large enough. □

Putting together (2.3), (2.1), and (2.2), we obtain

$$\begin{aligned}
&\mathbb{P}[(0.99n)^{1/2}s_k(G) \leqslant e(G)+k^2] \\
&\quad\geqslant \mathbb{P}\Big[(0.99n)^{1/2}s_k(G) \leqslant (0.99n)^{1/2}\Big(\sqrt{n}(k-1)+\frac{n}{2}\Big) \\
&\qquad\qquad\qquad\qquad \text{and } \frac{1-\delta}{2}\binom{n}{2}+k^2 \leqslant e(G)+k^2\Big] \\
&\quad\geqslant \mathbb{P}\Big[(0.99n)^{1/2}s_k(G) \leqslant (0.99n)^{1/2}\Big(\sqrt{n}(k-1)+\frac{n}{2}\Big)\Big] \\
&\qquad + \mathbb{P}\Big[\frac{1-\delta}{2}\binom{n}{2}+k^2 \leqslant e(G)+k^2\Big] - 1 \to 1.
\end{aligned}$$

That concludes the proof. □

In what follows we say that a sequence of random variables X_n converges almost surely (a.s.) towards X if $\mathbb{P}[\lim_{n\to\infty} X_n = X] = 1$. Let A_n be the adjacency matrix of an Erdős-Rényi random graph $G_n \sim G(n, \frac{1}{2})$. We denote by

$$\mu_n(x) := \frac{|\{\lambda_i(A_n)\colon\ \lambda_i(A_n) \leqslant x\}|}{n}$$

the empirical spectral distribution (ESD) of the eigenvalues of A_n. The fundamental Wigner semicircle law was first observed in 1955 by Wigner in [11] for certain special classes of random matrices arising in quantum mechanics. It states that $\mu_n(\sqrt{n}x)$ converges to $\mu(x)$ almost surely, where

$$\mu(x) = \begin{cases} \dfrac{2}{\pi}(1-x^2)^{1/2} & \text{if } |x| \leqslant 1, \\ 0 & \text{otherwise.} \end{cases}$$

That is, the semicircle law ensures weak convergence of the ESD to μ. From this fact it is possible to provide convergence for the sum of eigenvalues within a given range as we show next. To this end, let $s(t, G)$ be the sum of the adjacency eigenvalues of G larger than or equal to $t\sqrt{n}$, i.e.

$$s(t,G) = \sum_{\lambda_i \geqslant t\sqrt{n}} \lambda_i(A_G) = \sum_{\lambda_i \geqslant t} \lambda_i\Big(\frac{1}{\sqrt{n}}A_G\Big).$$

Proposition 2.1. *If $G_n \sim G(n, \frac{1}{2})$, then $(s(t, G_n))/n^{3/2}$ converges almost surely to $2(1-t^2)^{3/2}/(3\pi)$.*

P r o o f. If A_n is the adjacency matrix of G_n, denote by μ_n the ESD of $A_n/\sqrt{n}$.

Claim 2. For any bounded measurable function f and any $a, b \in [-1, 1]$ we have that $\int_a^b f\mu_n \overset{\text{a.s.}}{\to} \int_a^b f\mu$ almost surely.

P r o o f. By the semicircle law, we have pointwise convergence in $[a, b]$ almost surely. Let M be a bound such that $\max\{|f\mu_n|, |f\mu|\} \leqslant M$. By Egorov's Theorem, for any $\varepsilon > 0$ we can find a closed set $F \subset [a, b]$ such that the Lebesgue measure $\nu(\overline{F}) < \varepsilon/4M$ and $f\mu_n$ converges uniformly to $f\mu$ in F almost surely, i.e., for every $\varepsilon > 0$ there is N such that if $n \geqslant N$, then $|f(x)\mu_n(x) - f(x)\mu(x)| < \varepsilon/4$ for all $x \in F$ almost surely. We can write for $n \geqslant N$

$$\begin{aligned}
\left|\int_a^b f\mu_n - \int_a^b f\mu\right| &= \left|\int_F f\mu_n - \int_a^b f\mu\right| + \left|\int_{\overline{F}} f\mu_n\right| \\
&< \left|\int_F f\mu_n - \int_a^b f\mu\right| + \frac{\varepsilon}{4} \\
&< \left|\int_F f\mu_n - \int_F f\mu\right| + \left|\int_F f\mu - \int_a^b f\mu\right| + \frac{\varepsilon}{4} \\
&< \nu(F)\frac{\varepsilon}{4} + \left|\int_F f\mu - \int_a^b f\mu\right| + \frac{\varepsilon}{4} \\
&= \nu(F)\frac{\varepsilon}{4} + \left|\int_{\overline{F}} f\mu\right| + \frac{\varepsilon}{4} \\
&< \nu(F)\frac{\varepsilon}{4} + \frac{\varepsilon}{2} < \varepsilon, \quad \text{almost surely.}
\end{aligned}$$

That finishes the proof of the claim. □

Notice that the semicircle law gives only a limit distribution and does not describe the behavior of the largest eigenvalues. However, the results in [2] imply that $\lambda_1(G_n) = O(n)$ and $|\lambda_i| < \sqrt{n} + O(n^{1/3}\log n)$ for $i \geqslant 2$ almost surely. Thus, we can write

$$s(t, G_n) = \sqrt{n} + O(n^{1/3}\log n) + \sum_{\substack{\lambda_i \geqslant t \\ i \neq 1}} \lambda_i(A_n)$$

almost surely. Together with Claim 2, that gives us

$$\frac{1}{n}\sum_{\lambda_i \geqslant t} \lambda_i\Big(\frac{1}{\sqrt{n}}A_n\Big) \overset{\text{a.s.}}{=} \int_t^1 x\mu_n \overset{\text{a.s.}}{\to} \int_t^1 x\mu = \int_t^1 x\frac{2}{\pi}(1-x^2)^{1/2}\,\mathrm{d}x = \frac{2}{3\pi}(1-t^2)^{3/2}.$$

That means we have

$$\frac{s(t, G_n)}{n^{3/2}} = \frac{1}{n^{3/2}}\sum_{\lambda_i \geqslant t} \lambda_i(A_n) \overset{\text{a.s.}}{=} \frac{1}{n}\sum_{\lambda_i \geqslant t} \lambda_i\Big(\frac{1}{\sqrt{n}}A_n\Big) \overset{\text{a.s.}}{\to} \frac{2}{3\pi}(1-t^2)^{3/2},$$

as required. □

The previous result allows us to upper bound the partial sum of eigenvalues in a given range, as stated below.

Theorem 2.2. *For a random graph $G_n \sim G(n, \frac{1}{2})$ we have*

$$s(t, G_n) \leqslant \frac{2}{3\pi} n^{3/2} \left(\frac{e(G)}{\binom{n}{2}} + \frac{\left(1 - t^2\right)^3}{2} + o(1) \right)$$

asymptotically almost surely.

P r o o f. It is enough to show that for any constant $D > 0$ we have

$$\lim_{n \to \infty} \mathbb{P}\left[s(t, G_n) \leqslant \frac{2}{3\pi} n^{3/2} \left(\frac{e(G)}{\binom{n}{2}} + \frac{(1 - t^2)^3}{2} + D \right) \right] = 1.$$

To this end, we define $x = (1 - t^2)^{3/2}$ and $c = 2/(3\pi)$. Let $G_n \sim G(n, \frac{1}{2})$. By Proposition 2.1 for every $\varepsilon > 0$ we have

$$\mathbb{P}\left[\left| \frac{s(t, G_n)}{c n^{3/2}} - x \right| < \varepsilon \right] \to 1$$

as $n \to \infty$. This implies that for every $\varepsilon > 0$ we have

$$\mathbb{P}\left[\frac{s(t, G_n)}{c n^{3/2}} \leqslant x + \varepsilon \right] \to 1 \tag{2.4}$$

as $n \to \infty$. We will use the fact that the expected number of edges in G_n is $\frac{1}{2}(1 - \delta)\binom{n}{2}$, and that by the Hoeffding inequality [4], for any given $\delta > 0$ we have

$$\mathbb{P}\left(\frac{1 - \delta}{2} \binom{n}{2} \leqslant e(G_n) \right) \to 1 \tag{2.5}$$

as $n \to \infty$. We need the following.

Claim 3. For any $D > 0$ there exist $\varepsilon > 0$ and $\delta > 0$ such that $x + \varepsilon \leqslant \frac{1}{2}(1 - \delta + x^2) + D$.

P r o o f. As a polynomial in x, consider $f(x) := x^2/2 - x - \varepsilon + \frac{1}{2}(1 - \delta) + D$. This polynomial has discriminant $\Delta = 2\varepsilon + \delta - 2D$, which can be made negative for suitable choices of ε and δ. Thus $f(x) > 0$ for all x and the claim follows. □

Finally, we can fix ε and δ given by the claim and apply equations (2.5), (2.4), and Bonferroni's inequality to obtain

$$\begin{aligned}
&\mathbb{P}\left[\frac{s(t,G_n)}{cn^{3/2}} \leqslant \frac{e(G)}{\binom{n}{2}} + \frac{(1-t^2)^3}{2} + D\right] \\
&\quad \geqslant \mathbb{P}\left[\frac{s(t,G_n)}{cn^{3/2}} \leqslant x+\varepsilon \text{ and } \frac{1-\delta+x^2}{2} + D \leqslant \frac{e(G)}{\binom{n}{2}} + \frac{x^2}{2} + D\right] \\
&\quad \geqslant \mathbb{P}\Big[\frac{s(t,G_n)}{cn^{3/2}} \leqslant x+\varepsilon\Big] + \mathbb{P}\left[\frac{1-\delta+x^2}{2} + D \leqslant \frac{e(G)}{\binom{n}{2}} + \frac{x^2}{2} + D\right] - 1 \\
&\quad \to \mathbb{P}\left[\frac{1-\delta}{2} \leqslant \frac{e(G)}{\binom{n}{2}}\right] \to 1
\end{aligned}$$

as $n \to \infty$. That finishes the proof. □

3. Final remarks

We can find graphs where the bound from Theorem 2.1 is tighter than bound (1.1). This is possible because Theorem 2.1 accounts the number of edges, whereas bound (1.1) deals with general graphs. For example, the star S has spectrum $\{\sqrt{n-1}, 0, \ldots, 0, -\sqrt{n-1}\}$, and thus $s_1(S) < \sqrt{n}$ for all k. Notice that Theorem 2.1 implies $s_k(S) \lesssim \sqrt{n} + (k^2-1)/\sqrt{n}$ for all k, whereas (1.1) is bigger than n.

Furthermore, if we fix $k = cn$ for a natural number c, Theorem 2.1 ensures that $s_k \leqslant (e(G) + (cn)^2)/(0.99n)^{1/2} \sim n^{3/2}$. On the other hand, inequality (1.1) gives

$$s_k \leqslant \frac{cn}{2}(1+\sqrt{n}) \sim n^{3/2}.$$

That implies that the bound from our result that holds for almost all graphs matches the deterministic bound asymptotically.

We can use Theorem 2.2 to get an estimation for a bound on energy graphs. We use that the expected number of edges in $G(n, \frac{1}{2})$ is $\frac{1}{2}\binom{n}{2}$. Also using the notation of Theorem 2.2, we note that the energy of a graph can be written as

$$E(G) = 2s(0,G) < 2\left[\frac{2}{3\pi}n^{3/2}\left(\frac{e(G)}{\binom{n}{2}} + \frac{1}{2} + o(1)\right)\right] = \Big(\frac{4}{3\pi} + o(1)\Big)n^{3/2}$$

for almost all graphs, which agrees with (1.2).

We would like to mention that the bound from Theorem 2.1 can be stated in more general setting for $G(n,p)$, where p is not a constant. Notice that we run our proof for graphs sampled from $G(n,p)$ when p is a constant and in this case

the number of edges is typically of order n^2. In this regime the upper bound from Theorem 2.1 is of order $n^{3/2}$ which is the same order as of Nikiforov's bound (1.3). However, a more careful calculation using a suitable probability function $p = p(n)$ leads to a distribution where a typical graph has subquadratic number of edges which together with recent results on the eigenvalues of such graphs yields a similar bound in terms of the number of edges. After some routine calculations we can verify that the bound has order much smaller than $n^{3/2}$, which improves bound (1.3). Intuitively, that means that for a typical graph with subquadratic number of edges we have s_k much smaller than $n^{3/2}$.

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