TUM

Inequalities for the Number of Walks, the Spectral Radius, and the Energy of Graphs

Hanjo Täubig and Jeremias Weihmann

Technischer Bericht
Technische Universität München
Institut für Informatik

Inequalities for the Number of Walks, the Spectral Radius, and the Energy of Graphs

Hanjo Täubig*   Jeremias Weihmann*

Abstract

We unify and generalize several inequalities for the number w_k of walks of length k in graphs. The new inequalities use an arbitrary nonnegative weighting of the vertices. This allows an application of the theorems to subsets of vertices, i.e., these inequalities consider the number $w_k(S, S)$ of walks of length k that start at a vertex of a given vertex subset S and that end within the same subset. In particular, we show a weighted sandwich theorem for Hermitian matrices which generalizes a theorem by Marcus and Newman and which implies $w_{2a+c}(S, S) \cdot w_{2a+2b+c}(S, S) \leq w_{2a}(S, S) \cdot w_{2(a+b+c)}(S, S)$, a unification and generalization of inequalities by Lagarias et al. and by Dress & Gutman. Further, we show a theorem for nonnegative symmetric matrices that implies $w_{2\ell+p}(S, S)^k \leq w_{2\ell}(S, S)^{k-1} \cdot w_{2\ell+pk}(S, S)$, which is a unification and generalization of inequalities by Erdős & Simonovits, by Dress & Gutman, and by Ilić & Stevanović. Both results can be translated into corresponding forms for matrix or graph densities. In the end, these results are used to generalize lower bounds for the spectral radius and upper bounds for the energy of graphs.

1 Introduction

1.1 Notation and basic facts

Throughout the paper we assume that $\mathbb{N}$ denotes the set of nonnegative integers and $[n]$ is the set $\{1, \ldots, n\}$. Let $G = (V, E)$ be an undirected graph having n vertices, m edges and adjacency matrix A. We investigate (the number of) walks, i.e., sequences of vertices, where each pair of consecutive vertices is connected by an edge. Nodes and edges can be used repeatedly in the same walk. The length k of a walk is counted in terms of edges. For $k \in \mathbb{N}$ and $x, y \in V$, we denote by $w_k(x, y)$ the number of walks of length k that start at vertex x and end at vertex y. Since the graph is undirected we know that $w_k(x, y) = w_k(y, x)$. By $w_k(x) = \sum_{y \in V} w_k(x, y)$ we denote the number of all walks of length k that start at node x. Consequently, $w_k = \sum_{x \in V} w_k(x)$ denotes the total number of walks of length k.

It is a well known fact that the (i, j)-entry of A^k is the number of walks of length k that start at vertex i and end at vertex j (for all $k \geq 0$). Another fundamental observation about the number of walks is that in a graph $G = (V, E)$ for all vertices $x, z \in V$ holds $w_{k+\ell}(x, z) = \sum_{y \in V} w_k(x, y) \cdot w_\ell(y, z)$.

1.2 Motivation and related work

1.2.1 Inequalities for the number of walks

In a paper by Feige, Kortsarz, and Peleg [FKP01] on approximating the Dense k-Subgraph Problem the following observation was used: In a graph with n vertices and average degree $\bar{d}$, there exist two vertices v_i, v_j such that $\bar{d}^k/n \leq w_k(v_i, v_j)$. In the proof, they remark that this lemma would also follow from the following global statement: The number of walks of length k in a graph of

---

*Institut für Informatik, Technische Universität München, D-85748 Garching, Germany, {taeubig,weihmann}@in.tum.de

average degree $\overline{d}$ can be bounded from below by $n \cdot \overline{d}^k \leq w_k$. For a partial proof they referred to a paper by Alon, Feige, Wigderson, and Zuckerman [AFWZ95] that only covers the case of *even* values for k. However, several years before it had been noticed in a paper by Erdős and Simonovits (and actually Godsil, see [ES82]) that this inequality can be proven for all k using the results of Mulholland and Smith [MS59, MS60], Blakley and Roy [BR65], and London [Lon66]. Recently, we also found an article by Blakley and Dixon [BD66] that implies this result. Since $\overline{d} = 2m/n = w_1/w_0$, we can write the inequality in the following form:

Theorem 1 (Erdős & Simonovits). *In undirected graphs, the following inequality holds for $k \in \mathbb{N}$:*

$$w_k \geq n\overline{d}^k = n\left(\frac{w_1}{w_0}\right)^k \qquad or \qquad w_1^k \leq w_0^{k-1} w_k.$$

Lagarias, Mazo, Shepp, and McKay [LMSM83] posed the question for which numbers $r, s \in \mathbb{N}$ the inequality $w_r \cdot w_s \leq n \cdot w_{r+s}$ holds for all graphs. A little later, they proved the inequality for the case of an even sum $r + s$ [LMSM84]. Hence, it could be stated in the following way:

Theorem 2 (Lagarias et al.). *In undirected graphs holds for all $a, b \in \mathbb{N}$:*

$$w_{2a+b} \cdot w_b \leq w_0 \cdot w_{2(a+b)}.$$

Furthermore, Lagarias et al. presented counterexamples whenever $r + s$ is odd [LMSM84]; but they noted without proof, that for any graph G there is a constant c, s.t. for all $r, s \geq c$ the inequality is valid.

Dress and Gutman [DG03] reported the following inequality:

Theorem 3 (Dress & Gutman). *In undirected graphs holds for all $a, b \in \mathbb{N}$:*

$$w_{a+b}^2 \leq w_{2a} \cdot w_{2b}.$$

1.2.2 The spectral radius

Collatz and Sinogowitz [CS57] proved that the average degree $\overline{d} = 2m/n \leq \lambda_1$ is a lower bound for the largest eigenvalue of the adjacency matrix. Hofmeister [Hof88, Hof94] later showed that $\sum_{v \in V} d_v^2 / n \leq \lambda_1^2$. These bounds are equivalent to $w_1/w_0 \leq \lambda_1$ and $w_2/w_0 \leq \lambda_1^2$.

Three other publications with lower bounds, namely $\sum_{v \in V} w_2(v)^2 / \sum_{v \in V} d_v^2 \leq \lambda_1^2$ [YLT04], $\sum_{v \in V} w_3(v)^2 / \sum_{v \in V} w_2(v)^2 \leq \lambda_1^2$ [HZ05], and $\sum_{v \in V} w_{k+1}(v)^2 / \sum_{v \in V} w_k(v)^2 \leq \lambda_1^2$ [HTW07] consider the sum of squares of walk numbers, but do not mention the corresponding number of walks of the double length ($w_4/w_2 \leq \lambda_1^2$, $w_6/w_3 \leq \lambda_1^2$ and $w_{2k+2}/w_{2k} \leq \lambda_1^2$).

These results were generalized by Nikiforov [Nik06] to $\frac{w_{k+r}}{w_k} \leq \lambda_1^r$ for all $r \geq 1$ and *even* numbers $k \geq 0$.[1] In particular, this implies a bound using the average number of walks of length k and a bound regarding the growth factor for odd / even walk lengths: $\frac{w_r}{n} \leq \lambda_1^r$ and $\frac{w_{2\ell+1}}{w_{2\ell}} \leq \lambda_1$ which also contains the bound of Collatz and Sinogowitz as a special case. As an upper bound for λ_1, Nikiforov [Nik06] proved that for all $r \geq 1$ and $k \geq 0$: $\lambda_1^r \leq \max_{v \in V} \frac{w_{k+r}(v)}{w_k(v)}$.

Nosal [Nos70] proved another lower bound for the spectral radius using the square root of the maximum degree: $\sqrt{\Delta} \leq \lambda_1$ which is generalized in the second part of this paper. Those bounds provide an opportunity to compute lower bounds for other graph measures such as the chromatic number (using an inequality of Hoffman $1 - \lambda_1/\lambda_n \leq \chi(G)$, see [Hof70]), the clique number (using an inequality of Wilf $n/(n - \lambda_1) \leq \omega$, see [Wil86]) or network-related properties like the epidemic threshold ($1/\lambda_1$, see [CWW$^+$08]).

For a survey of bounds of the largest eigenvalue, see [CR90]. More information on applications of graph spectra can be found in [Cve09, Cio11, VM11].

---

[1] Note that Nikiforov used *odd* values for k which is due to the fact that he counted vertices instead of edges for defining w_k.

1.3 The spectral approach to the number of walks

We now briefly review the properties of the eigenvalues and eigenvectors of the graphs adjacency matrix which were first studied by Collatz and Sinogowitz [CS57]. In particular, they investigated relations between the spectral index and the minimum, average, and maximum degree of the graph. Connections to the more general numbers of walks were investigated by Cvetković [Cve70, Cve71], later also by Harary and Schwenk [HS79]. Classic books on spectral graph theory are, e.g., [CDS79, CDGT88, Chu97, CRS97].

Let λ_i $(1 \leq i \leq n)$ denote the eigenvalues of the adjacency matrix A. Since A is real and symmetric, all eigenvalues of A are real numbers and A is diagonalizable by an orthogonal matrix, i.e., there is an orthogonal matrix U, s.t. $U^T A U = D$ is a diagonal matrix of the eigenvalues $D = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Accordingly, the adjacency matrix can be written as $A = U D U^T$ where the columns of U are formed by an orthonormal basis of eigenvectors (orthogonal matrices satisfy $U^{-1} = U^T$). We also define $B_i = \sum_{x=1}^{n} u_{xi}$ as an abbreviation for the column sums of U.

The number of walks of length k from vertex i to vertex j is exactly the (i, j)-entry of the matrix power $A^k = (U D U^T)^k = U D^k U^T$. The total number of walks of length k is $w_k = \langle \mathbf{1}_n, A^k \mathbf{1}_n \rangle = \left\langle \mathbf{1}_n, \left(U D U^T \right)^k \mathbf{1}_n \right\rangle = \langle \mathbf{1}_n, \left(U D^k U^T \right) \mathbf{1}_n \rangle$, where $\langle \ldots \rangle$ denotes the inner product of the given vectors and $\mathbf{1}_n$ is the vector with n entries each of which is 1. The number of walks between given vertices is therefore

$$w_k(x, y) \quad = \quad \sum_{i=1}^{n} u_{xi} u_{yi} \lambda_i^k$$

while the number of walks starting at a given vertex is

$$w_k(x) = \sum_{y=1}^{n} \sum_{i=1}^{n} u_{xi} u_{yi} \lambda_i^k = \sum_{i=1}^{n} \left(u_{xi} \lambda_i^k \sum_{y=1}^{n} u_{yi} \right) = \sum_{i=1}^{n} u_{xi} B_i \lambda_i^k.$$

Then, the total number of walks is given by

$$w_k = \sum_{i=1}^{n} \left(\sum_{x=1}^{n} u_{xi} \right)^2 \lambda_i^k = \sum_{i=1}^{n} B_i^2 \lambda_i^k.$$

From the diagonalization $U^T A U = D = \mathrm{diag}(\lambda_1 \ldots \lambda_n)$ it can be seen that the i-th eigenvalue λ_i and (unit) eigenvector $(u_{1i} \ldots u_{ni})^T$ satisfy $\lambda_i = \sum_{(x,y) \in E} u_{xi} u_{yi}$. An even more general statement follows from $U^T A^k U = (U^T A U)^k = D^k = \mathrm{diag}(\lambda_1^k \ldots \lambda_n^k)$: $\lambda_i^k = \sum_{x \in V, y \in V} w_k(x, y) u_{xi} u_{yi}$. In the same way it can be shown that for all $i \neq j$ holds $0 = \sum_{(x,y) \in E} u_{xi} u_{yj}$ and $0 = \sum_{x \in V, y \in V} w_k(x, y) u_{xi} u_{yj}$.

Since $U^T A U = U^{-1} A U = D$, the trace of A equals the trace of D. Due to the fact, that the entries of the main diagonal are the numbers of closed walks starting and ending at the respective nodes, we get $\sum_{i=1}^{n} \lambda_i = 0$ and $\sum_{i=1}^{n} \lambda_i^2 = 2m$. For bipartite graphs we get even more restrictions (there are no closed walks of odd length), i.e., $\sum_{i=1}^{n} \lambda_i^{2k+1} = 0$ which goes with the fact that the spectrum of the graph is symmetric.

2 Inequalities for the Number of Walks

2.1 The Weighted Sandwich Theorem – A unifying generalization of inequalities by Lagarias et al. and Dress/Gutman

In this section, we assume the more general case where A is a Hermitian matrix. Then the sum of all entries is a real number. In a more general view, also the sum of all entries for any principal submatrix is a real number (in particular this applies to each entry on the main diagonal). In an even more general consideration, it is also possible to assign a certain real weight to each index

(vertex), and to multiply rows and columns by this chosen scaling vector $\vec{s}$ which again yields a real number as the sum of all entries. Of course, the same applies to the powers of the matrix. Also the eigenvalues are all real. Further, A can be diagonalized by a unitary matrix U consisting of n orthonormal eigenvectors of A, i.e., $A = UDU^*$, where U^* is the conjugate transpose of U and D is the diagonal matrix containing the corresponding (real) eigenvalues λ_i. For any real weight vector $\vec{s}$, we define $B_{i,\vec{s}} = \sum_{x=1}^{n} s_x u_{xi}$ as an abbreviation for the weighted column sums of U. We know that $A^k = (UDU^*)^k = UD^kU^*$. Let $\bar{c}$ denote the complex conjugate of $c \in \mathbb{C}$. Now, we use the following generalized definitions for entry sums of matrix powers (instead of adjacency matrices and numbers of walks):

$$w_k(x,y) = \left(A^k\right)_{(x,y)} = \sum_{i=1}^{n} u_{xi}\bar{u}_{yi}\lambda_i^k.$$

For some index x, we define $w_{k,\vec{s}}(x)$ to be the weighted sum of the terms $w_k(x,y)$ for all $y \in [n]$:

$$w_{k,\vec{s}}(x) = \sum_{y=1}^{n} s_y w_k(x,y) = \sum_{y=1}^{n} s_y \sum_{i=1}^{n} u_{xi}\bar{u}_{yi}\lambda_i^k = \sum_{i=1}^{n}\left(u_{xi}\lambda_i^k \sum_{y=1}^{n} s_y \bar{u}_{yi} \right) = \sum_{i=1}^{n} u_{xi}\bar{B}_{i,\vec{s}}\lambda_i^k$$

Then, the total (again weighted) sum of the entries is

$$w_{k,\vec{s}} = \sum_{x=1}^{n} s_x w_{k,\vec{s}}(x) = \sum_{x=1}^{n} s_x \sum_{i=1}^{n} u_{xi}\bar{B}_{i,\vec{s}}\lambda_i^k = \sum_{i=1}^{n}\left(\bar{B}_{i,\vec{s}}\lambda_i^k \sum_{x=1}^{n} s_x u_{xi} \right) = \sum_{i=1}^{n} B_{i,\vec{s}}\bar{B}_{i,\vec{s}}\lambda_i^k$$

Theorem 4 (Weighted Sandwich Theorem). *For all $a, b, c \in \mathbb{N}$ and all weight vectors $\vec{s} \in \mathbb{R}^n$ holds:*

$$w_{2a+c,\vec{s}} \cdot w_{2a+2b+c,\vec{s}} \leq w_{2a,\vec{s}} \cdot w_{2(a+b+c),\vec{s}}$$

Proof. Consider the difference of both sides of the inequality:

$$\sum_{i=1}^{n} B_{i,\vec{s}}\bar{B}_{i,\vec{s}}\lambda_i^{2a} \sum_{j=1}^{n} B_{j,\vec{s}}\bar{B}_{j,\vec{s}}\lambda_j^{2(a+b+c)} - \sum_{i=1}^{n} B_{i,\vec{s}}\bar{B}_{i,\vec{s}}\lambda_i^{2a+c} \sum_{j=1}^{n} B_{j,\vec{s}}\bar{B}_{j,\vec{s}}\lambda_j^{2a+2b+c}$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} B_{i,\vec{s}}\bar{B}_{i,\vec{s}}B_{j,\vec{s}}\bar{B}_{j,\vec{s}}\left(\lambda_i^{2a}\lambda_j^{2(a+b+c)} - \lambda_i^{2a+c}\lambda_j^{2a+2b+c} \right)$$

$$= \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} B_{i,\vec{s}}\bar{B}_{i,\vec{s}}B_{j,\vec{s}}\bar{B}_{j,\vec{s}}\left(\lambda_i^{2a}\lambda_j^{2(a+b+c)} - \lambda_i^{2a+c}\lambda_j^{2a+2b+c} + \lambda_j^{2a}\lambda_i^{2(a+b+c)} - \lambda_j^{2a+c}\lambda_i^{2a+2b+c} \right)$$

$$= \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} B_{i,\vec{s}}\bar{B}_{i,\vec{s}}B_{j,\vec{s}}\bar{B}_{j,\vec{s}}\lambda_i^{2a}\lambda_j^{2a}\left(\lambda_j^{2(b+c)} - \lambda_i^c\lambda_j^{2b+c} + \lambda_i^{2(b+c)} - \lambda_j^c\lambda_i^{2b+c} \right)$$

$$= \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} B_{i,\vec{s}}\bar{B}_{i,\vec{s}}B_{j,\vec{s}}\bar{B}_{j,\vec{s}}\lambda_i^{2a}\lambda_j^{2a}\left(\lambda_j^{2b+c} - \lambda_i^{2b+c} \right)\left(\lambda_j^c - \lambda_i^c \right)$$

Note that the product of a complex number and its conjugate is a nonnegative real number. Therefore, each term within the last line must be nonnegative, since $(B_{i,\vec{s}}\bar{B}_{i,\vec{s}})$, $(B_{j,\vec{s}}\bar{B}_{j,\vec{s}})$, λ_i^{2a}, and λ_j^{2a} are all nonnegative, and $(\lambda_j^{2b+c} - \lambda_i^{2b+c})$ and $(\lambda_j^c - \lambda_i^c)$ must have the same sign. $\square$

Setting $\vec{s}$ to the characteristic vector of an index subset $S \subseteq [n]$ gives a relation for the sum of entries restricted to the corresponding principal submatrix of the matrix power. In this case, we denote the sum of the corresponding matrix entries by $w_k(S,S)$. Note, that this is different compared to considering powers of the principle submatrix.

4

Corollary 5. *For all $a, b, c \in \mathbb{N}$ and all subsets $S \subseteq [n]$ holds:*

$$w_{2a+c}(S, S) \cdot w_{2a+2b+c}(S, S) \leq w_{2a}(S, S) \cdot w_{2(a+b+c)}(S, S)$$

Applied to adjacency matrices of undirected graphs (where the matrix entries count the number of walks of a certain length between vertices), the sum is restricted to the walks between vertices in the chosen subset. The difference is that in the first case only the start and end vertices must be in S, while in the second case only walks are counted where also the intermediate vertices come from the subset S.

By setting $S = [n]$ ($\vec{s} = \mathbf{1}_n$), we get the sandwich theorem for the total sum of the matrix entries:

$$0 \leq \sum_{i,j} A^{2a}_{(i,j)} \cdot \sum_{i,j} A^{2(a+b+c)}_{(i,j)} - \sum_{i,j} A^{2a+c}_{(i,j)} \cdot \sum_{i,j} A^{2a+2b+c}_{(i,j)}$$

This special case of the statement had already been obtained by Marcus and Newman [MN62].

In the case where S only contains one index (or vertex) v, this yields the statement for the entries on the main diagonal (which correspond to closed walks in the case of adjacency matrices):

$$0 \leq A^{2a}_{(v,v)} \cdot A^{2(a+b+c)}_{(v,v)} - A^{2a+c}_{(v,v)} \cdot A^{2a+2b+c}_{(v,v)}$$

Generalized graph density: For a graph G having $n \geq 2$ vertices and m edges the density ρ is defined as the fraction of present edges: $\rho = \frac{m}{\binom{n}{2}} = \frac{2m}{n(n-1)}$. Accordingly, a generalized k-th order density can be defined (see [Kos05]) using the number of length-k walks: $\rho_k = \frac{w_k}{n(n-1)^k}$ (with $\rho_0 = 1$ and $\rho_1 = \rho$). The Sandwich Theorem directly implies the following inequality:

$$\frac{w_{2a+c} \cdot w_{2a+2b+c}}{[n(n-1)^{2a+c}] \cdot [n(n-1)^{2a+2b+c}]} \leq \frac{w_{2a} \cdot w_{2(a+b+c)}}{[n(n-1)^{2a}] \cdot [n(n-1)^{2(a+b+c)}]}$$

Corollary 6. *For all $a, b, c \in \mathbb{N}$ holds:*

$$\rho_{2a+c} \cdot \rho_{2a+2b+c} \leq \rho_{2a} \cdot \rho_{2(a+b+c)}$$

The same method can be applied for more general matrices, e.g., for adjacency matrices of graphs where loops are allowed and the corresponding denominator is n^{k+1} instead of $n(n-1)^k$.

2.2 A unifying generalization of the inequalities by Erdős/Simonovits, Dress/Gutman, and Ilić/Stevanović

We now show a generalization of Theorem 1 (the inequality of Erdős and Simonovits) which is at the same time another generalization of Theorem 3 (the inequality of Dress and Gutman). As we will see, the new theorem also generalizes two inequalities by Ilić and Stevanović. While our first proof [HKM+11] used a theorem of Blakley and Roy [BR65], we later [HKM+12] found a paper by Blakley and Dixon [BD66] that allows a more direct proof using the following theorem:

Theorem 7 (Blakley & Dixon [BD66]). *For any positive integer q, nonnegative real n-vector u and nonnegative real symmetric $n \times n$-matrix S holds:*

$$\langle u, Su \rangle^{q+1} \leq \langle u, u \rangle^q \langle u, S^{q+1} u \rangle.$$

Now, we apply Theorem 7 to a nonnegative matrix $S = A^p$ and a nonnegative vector u consisting of the values $w_{\ell, \vec{s}}(v)$ (cf. definitions before the Weighted Sandwich Theorem), and setting $q = k - 1$ (note that for $\langle u, u \rangle \neq 0$ and $q \in \{-1, 0\}$ both sides are equal). To satisfy the restrictions, it is sufficient to assume that A and $\vec{s}$ are nonnegative.

Theorem 8. *For every nonnegative real symmetric matrix A, nonnegative weight vector $\vec{s}$, and $k, \ell, p \in \mathbb{N}$, the following inequality holds if $k \geq 2$ or $w_{2\ell,\vec{s}} > 0$:*

$$w_{2\ell+p,\vec{s}}^k \leq w_{2\ell,\vec{s}}^{k-1} \cdot w_{2\ell+pk,\vec{s}}.$$

For all matrices with $w_{2\ell,\vec{s}} > 0$, this is equivalent to

$$\left(\frac{w_{2\ell+p,\vec{s}}}{w_{2\ell,\vec{s}}} \right)^k \leq \frac{w_{2\ell+pk,\vec{s}}}{w_{2\ell,\vec{s}}} \qquad and \qquad \left(\frac{w_{2\ell+p,\vec{s}}}{w_{2\ell,\vec{s}}} \right)^{k-1} \leq \frac{w_{2\ell+pk,\vec{s}}}{w_{2\ell+p,\vec{s}}}.$$

If the matrix is the adjacency matrix of a graph $G = (V, E)$ and $\vec{s}$ is the characteristic vector of a vertex subset $S \in V$, then $\vec{w}_{\ell,\vec{s}}(v)$ is the vector of walks of length ℓ that start at vertex v and end at a vertex of this subset S. This way, each of the length-k walks from vertex x to vertex y is multiplied by $w_{\ell,\vec{s}}(x)$ and $w_{\ell,\vec{s}}(y)$, i.e., the number of length-ℓ walks starting at a vertex of S and ending at x and the number of length-ℓ walks starting at y and ending at a vertex of S, resp. This results in counting the walks of length k that are extended at the beginning and at the end by all possible walks of length ℓ, i.e., walks of length $k + 2\ell$, that start and end at vertices of S (where the intermediate vertices may also come from $V \setminus S$).

Corollary 9. *For every graph $G = (V, E)$, vertex subset $S \subseteq V$, and $k, \ell, p \in \mathbb{N}$, the following inequality holds if $k \geq 2$ or $w_{2\ell}(S, S) > 0$:*

$$w_{2\ell+p}(S, S)^k \leq w_{2\ell}(S, S)^{k-1} \cdot w_{2\ell+pk}(S, S).$$

For all graphs with $w_{2\ell}(S, S) > 0$, this is equivalent to

$$\left(\frac{w_{2\ell+p}(S, S)}{w_{2\ell}(S, S)} \right)^k \leq \frac{w_{2\ell+pk}(S, S)}{w_{2\ell}(S, S)} \qquad and \qquad \left(\frac{w_{2\ell+p}(S, S)}{w_{2\ell}(S, S)} \right)^{k-1} \leq \frac{w_{2\ell+pk}(S, S)}{w_{2\ell+p}(S, S)}.$$

For $\ell = 0$, we obtain an inequality which compares the average number of walks (per vertex) of lengths p and pk:

Corollary 10. *For every graph $G = (V, E)$, vertex subset $S \subseteq V$ with $|S| \geq 1$, and $k, p \in \mathbb{N}$, the following inequalities hold:*

$$w_p(S, S)^k \leq |S|^{k-1} w_{pk}(S, S) \qquad and \qquad \left(\frac{w_p(S, S)}{|S|} \right)^k \leq \frac{w_{pk}(S, S)}{|S|}.$$

As a special case ($\ell = 0$ and $p = 1$) we get $w_1(S, S)^k \leq w_k(S, S) \cdot w_0(S, S)^{k-1}$ where $w_1(S, S)$ is the number of edges in the subgraph induced by S and $w_1(S, S)/w_0(S, S) = w_1(S, S)/|S|$ is the average degree in this subgraph.

If the chosen subset S contains only a single vertex v, then we get a statement about closed walks using v:

Corollary 11. *For every graph $G = (V, E)$, vertex $v \in V$, and $k, \ell, p \in \mathbb{N}$, the following inequality holds if $k \geq 2$ or $w_{2\ell}(v, v) > 0$:*

$$w_{2\ell+p}(v, v)^k \leq w_{2\ell+pk}(v, v) \cdot w_{2\ell}(v, v)^{k-1}.$$

Under the respective conditions $w_{2\ell}(v, v) > 0$ and $w_{2\ell+p}(v, v) > 0$ this is equivalent to

$$\left(\frac{w_{2\ell+p}(v, v)}{w_{2\ell}(v, v)} \right)^k \leq \frac{w_{2\ell+pk}(v, v)}{w_{2\ell}(v, v)} \qquad and \qquad \left(\frac{w_{2\ell+p}(v, v)}{w_{2\ell}(v, v)} \right)^{k-1} \leq \frac{w_{2\ell+pk}(v, v)}{w_{2\ell+p}(v, v)}$$

If the subset S includes all of the vertices, then we get the following result:

Corollary 12. *For all graphs and $k, \ell, p \in \mathbb{N}$ the following inequality holds if $k \geq 2$ or $w_{2\ell} > 0$:*

$$w_{2\ell+p}^k \leq w_{2\ell}^{k-1} \cdot w_{2\ell+pk}.$$

For all graphs with $w_{2\ell} > 0$, this is equivalent to

$$\left(\frac{w_{2\ell+p}}{w_{2\ell}}\right)^k \leq \frac{w_{2\ell+pk}}{w_{2\ell}} \qquad \text{and} \qquad \left(\frac{w_{2\ell+p}}{w_{2\ell}}\right)^{k-1} \leq \frac{w_{2\ell+pk}}{w_{2\ell+p}}$$

Setting $k = 2$ leads to $w_{2\ell+p}^2 \leq w_{2\ell+2p} \cdot w_{2\ell}$ and therefore results in Theorem 3 published by Dress and Gutman. Furthermore, Corollary 12 is a generalization of the two inequalities

$$\frac{M_1}{n} \geq \frac{4m^2}{n^2} \qquad \text{and} \qquad \frac{M_2}{m} \geq \frac{4m^2}{n^2}$$

for the Zagreb indices M_1 and M_2 that were proposed by Ilić and Stevanović [IS09]. These bounds are just the same as

$$\frac{w_2}{w_0} \geq \frac{w_1^2}{w_0^2} \qquad \text{and} \qquad \frac{w_3/2}{w_1/2} \geq \frac{w_1^2}{w_0^2}.$$

Additionally, the theorem implies the following special case for $\ell = 0$, which is interesting on its own since it compares the average number of walks (per vertex) of lengths p and pk:

Corollary 13. *For graphs with at least one node and $k, p \in \mathbb{N}$, the following inequalities hold:*
$w_p^k \leq n^{k-1} w_{pk}$ *and* $\left(\frac{w_p}{n}\right)^k \leq \frac{w_{pk}}{n}$.

As a special case ($\ell = 0$ and $p = 1$) we get $w_1^k \leq w_k \cdot w_0^{k-1}$ which is (by $w_1/w_0 = 2m/n = \bar{d}$) exactly Theorem 1 reported by Erdős and Simonovits.

3 Lower Bounds For the Spectral Radius

3.1 The lower bound

In the following, we are considering powers of a nonnegative symmetric matrix A. The Perron-Frobenius Theorem guarantees that the spectral radius equals the largest eigenvalue. Hence, $[\lambda_1(A)]^k = \lambda_1(A^k)$. The Rayleigh-Ritz Theorem implies

$$\lambda_1(A) = \max_{||\mathbf{x}|| \neq 0} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}}.$$

For a vertex subset $S \subseteq V$ and a vertex $v \in V$, we define $w_\ell(S, v) = \sum_{s \in S} w_\ell(s, v) = \sum_{s \in S} w_\ell(v, s) = w_\ell(v, S)$ to be the number of walks of length ℓ from v to any vertex in S (or vice versa). Let $\vec{w}_\ell(S)$ denote the vector with entries $w_\ell(S, v)$ for all $v \in V$, then we conclude for a subset $S \subseteq V$ with $w_\ell(S) > 0$:

$$[\lambda_1(A)]^k = \lambda_1(A^k) \quad \geq \quad \frac{\vec{w}_\ell(S)^T A^k \vec{w}_\ell(S)}{\vec{w}_\ell(S)^T \vec{w}_\ell(S)} = \frac{w_{2\ell+k}(S, S)}{w_{2\ell}(S, S)}$$

Theorem 14. *For arbitrary graphs, the spectral radius of the adjacency matrix satisfies the following inequality:*

$$\lambda_1 \geq \max_{S \subseteq V, w_\ell(S) > 0} \sqrt[k]{\frac{w_{2\ell+k}(S, S)}{w_{2\ell}(S, S)}}$$

The case $\ell = 0$ and $S = \{v\}$ corresponds to the form $\lambda_1 \geq \max_{v \in V} \sqrt[k]{w_k(v, v)}$, i.e., this is an even more general form of the lower bound $\lambda_1 \geq \sqrt{\Delta}$ by Nosal [Nos70].

3.2 Monotonicity for even walk lengths

We now show that the new inequality for the spectral radius yields better bounds with increasing walk lengths if we restrict the walk lengths to even numbers. Correspondingly, we define a family of lower bounds in case $w_{2\ell}(S,S) > 0$:

$$F_{k,\ell}(S) = \sqrt[2k]{\frac{w_{2k+2\ell}(S,S)}{w_{2\ell}(S,S)}}$$

Lemma 15. *For $k, \ell, x, y \in \mathbb{N}$ with $k \geq 1$ holds*

$$\max_{S \subseteq V} F_{k+x, \ell+y}(S) \quad \geq \quad \max_{S \subseteq V} F_{k,\ell}(S)$$

Proof. To show $\max_{S \subseteq V} F_{k+x, \ell+y}(S) \geq \max_{S \subseteq V} F_{k,\ell}(S)$ it is sufficient to show $F_{k+x, \ell+y}(S) \geq F_{k,\ell}(S)$ for each $S \subseteq V$.

First we show monotonicity in k, i.e., $\sqrt[k+1]{\frac{w_{2(k+1)+2\ell}(S,S)}{w_{2\ell}(S,S)}} = F_{k+1,\ell}^2 \geq F_{k,\ell}^2 = \sqrt[k]{\frac{w_{2k+2\ell}(S,S)}{w_{2\ell}(S,S)}}$.

For the base case $k = 1$, it is sufficient to show that

$$\frac{w_{2(1+1)+2\ell}(S,S)}{w_{2\ell}(S,S)} \geq \left(\frac{w_{2+2\ell}(S,S)}{w_{2\ell}(S,S)}\right)^2.$$

This inequality is equivalent to $w_{4+2\ell}(S,S) \cdot w_{2\ell}(S,S) \geq w_{2+2\ell}(S,S)^2$ which follows from the Weighted Sandwich Theorem. What is left to show is

$$\frac{w_{2(k+2)+2\ell}(S,S)}{w_{2\ell}(S,S)} \bigg/ \frac{w_{2(k+1)+2\ell}(S,S)}{w_{2\ell}(S,S)} \geq \frac{w_{2(k+1)+2\ell}(S,S)}{w_{2\ell}(S,S)} \bigg/ \frac{w_{2k+2\ell}(S,S)}{w_{2\ell}(S,S)}$$

This inequality is equivalent to $w_{2(k+2)+2\ell}(S,S) \cdot w_{2k+2\ell}(S,S) \geq w_{2(k+1)+2\ell}(S,S)^2$ which again follows from the Weighted Sandwich Theorem.

Now we show monotonicity in ℓ, i.e., $\sqrt[k]{\frac{w_{2k+2(\ell+1)}(S,S)}{w_{2(\ell+1)}(S,S)}} = F_{k,\ell+1}^2 \geq F_{k,\ell}^2 = \sqrt[k]{\frac{w_{2k+2\ell}(S,S)}{w_{2\ell}(S,S)}}$. This is equivalent to $w_{2k+2(\ell+1)}(S,S) \cdot w_{2\ell}(S,S) \geq w_{2k+2\ell}(S,S) \cdot w_{2(\ell+1)}(S,S)$ which again follows from the Weighted Sandwich Theorem. $\square$

Theorem 8 (Corollaries 12 and 11) directly imply additional monotonicity results for our new bound, as well as for Nikiforov's bound:

$$\sqrt[p]{\frac{w_{2\ell+p}(S,S)}{w_{2\ell}(S,S)}} \quad \leq \quad \sqrt[pk]{\frac{w_{2\ell+pk}(S,S)}{w_{2\ell}(S,S)}} \qquad \text{which implies}$$

$$\sqrt[p]{\frac{w_{2\ell+p}(v,v)}{w_{2\ell}(v,v)}} \quad \leq \quad \sqrt[pk]{\frac{w_{2\ell+pk}(v,v)}{w_{2\ell}(v,v)}} \qquad \text{and}$$

$$\sqrt[p]{\frac{w_{2\ell+p}}{w_{2\ell}}} \quad \leq \quad \sqrt[pk]{\frac{w_{2\ell+pk}}{w_{2\ell}}}$$

In contrast to Lemma 15, these inequalities provide a monotonicity statement for certain *odd* walk lengths, too.

3.3 Generalized upper bounds for the energy of graphs

The total π-electron energy E_π plays a central role in the Hückel theory of theoretical chemistry. In the case that all molecular orbitals are occupied by two electrons this energy can be defined as $E_\pi = 2 \sum_{i=1}^{n/2} \lambda_i$. For bipartite graphs, this is equal to $\sum_{i=1}^{n} |\lambda_i|$ since the spectrum is symmetric. This motivated the definition of *graph energy* as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. First bounds for this quantity were given by McClelland [McC71]: $\sqrt{2m + n(n-1)|\det A|^{2/n}} \leq E(G) \leq \sqrt{2mn}$.

Later, several other bounds were published [Gut01]. A younger result is the following [HTW07]: the energy of a connected graph G with $n \geq 2$ vertices is bounded by

$$E(G) \leq \sqrt{\frac{\sum_{v \in V} w_{k+1}(v)^2}{\sum_{v \in V} w_k(v)^2}} + \sqrt{(n-1)\left(2m - \frac{\sum_{v \in V} w_{k+1}(v)^2}{\sum_{v \in V} w_k(v)^2}\right)}$$

We note that this corresponds to

$$E(G) \leq \sqrt{\frac{w_{2k+2}}{w_{2k}}} + \sqrt{(n-1)\left(2m - \frac{w_{2k+2}}{w_{2k}}\right)}$$

We now deduce a generalized bound from the lower bound for the spectral radius. Since $\lambda_1 \geq 0$ the definition of the graph energy can be written as

$$\begin{aligned}
E(G) &= \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \\
&\leq \lambda_1 + \sqrt{(n-1)\sum_{i=2}^{n} \lambda_i^2} \\
&\leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}
\end{aligned}$$

where the last two lines follow from the inequality $\left(\sum_{k=1}^{n} a_k\right)^2 \leq n \cdot \sum_{k=1}^{n} a_k^2$ and the fact $\sum_{i=1}^{n} \lambda_i^2 = 2m$.

Since the function $f(x) = x + \sqrt{(n-1)(2m - x^2)}$ has derivative $f'(x) = 1 - \frac{\sqrt{n-1}x}{\sqrt{2m-x^2}}$ and is therefore monotonically decreasing in the interval $\sqrt{2m/n} \leq x \leq \sqrt{2m}$ we have

$$\sqrt{2m} \geq \lambda_1 \geq F_{k,\ell}(V) \geq F_{1,0}(V) = \sqrt{\frac{w_2}{w_0}} \geq \sqrt{\frac{w_1}{w_0}} = \sqrt{\frac{2m}{n}}$$

which implies $f(\lambda_1) \leq f\left(F_{k,\ell}(V)\right)$ and thus

$$\begin{aligned}
E(G) &\leq f(\lambda_1) \leq f(G_{k,\ell}) \\
&\leq \sqrt[2k]{\frac{w_{2k+2\ell}}{w_{2\ell}}} + \sqrt{(n-1)\left(2m - \sqrt[k]{\frac{w_{2k+2\ell}}{w_{2\ell}}}\right)}
\end{aligned}$$

Similarly, we have

$$\sqrt{2m} \geq \lambda_1 \geq F_{k,\ell}(S) \geq F_{1,0}(S) = \sqrt{\frac{w_2(S,S)}{w_0(S,S)}} \geq \sqrt{\frac{w_1(S,S)}{w_0(S,S)}} = \sqrt{\frac{|E(G[S])|}{|S|}}$$

which implies for each set S having average degree of the induced subgraph $\overline{d}(G[S]) \geq \overline{d} = 2m/n$ that $f(\lambda_1) \leq f\left(F_{k,\ell}(S)\right)$ and thus

$$\begin{aligned}
E(G) &\leq f(\lambda_1) \leq f\left(F_{k,\ell}(S)\right) \\
&\leq \sqrt[2k]{\frac{w_{2k+2\ell}(S,S)}{w_{2\ell}(S,S)}} + \sqrt{(n-1)\left(2m - \sqrt[k]{\frac{w_{2k+2\ell}(S,S)}{w_{2\ell}(S,S)}}\right)}
\end{aligned}$$

Since $\frac{w_2(S,S)}{w_0(S,S)} \geq \frac{w_1(S,S)^2}{w_0(S,S)^2}$ (Sandwich Theorem), the same applies if $\frac{w_1(S,S)}{w_0(S,S)} = \overline{d}(G[S]) \geq \sqrt{\frac{2m}{n}}$.

For $S = \{v\}$, we get

$$\sqrt{2m} \geq \lambda_1 \geq F_{k,\ell}(v) \geq F_{1,0}(v) = \sqrt{\frac{w_2(v,v)}{w_0(v,v)}} = \sqrt{d_v}$$

9

which implies for each node v having degree $d_v \geq \bar{d} = 2m/n$ that $f(\lambda_1) \leq f(F_{k,\ell}(v))$ and thus

$$
\begin{aligned}
E(G) \quad &\leq \quad f(\lambda_1) \leq f\left(F_{k,\ell}(v)\right) \\
&\leq \quad \sqrt[2k]{\frac{w_{2k+2\ell}(v,v)}{w_{2\ell}(v,v)}} + \sqrt{(n-1)\left(2m - \sqrt[k]{\frac{w_{2k+2\ell}(v,v)}{w_{2\ell}(v,v)}}\right)}
\end{aligned}
$$

References

[AFWZ95] Noga Alon, Uriel Feige, Avi Wigderson, and David Zuckerman. Derandomized graph products. *Computational Complexity*, 5(1):60–75, March 1995.

[BD66] George R. Blakley and R. D. Dixon. Hölder type inequalities in cones. *Journal of Mathematical Analysis and Applications*, 14(1):1–4, April 1966.

[BR65] George R. Blakley and Prabir Roy. A Hölder type inequality for symmetric matrices with nonnegative entries. *Proceedings of the American Mathematical Society*, 16(6):1244–1245, December 1965.

[CDGT88] Dragoš M. Cvetković, Michael Doob, Ivan Gutman, and Aleksandar Torgašev. *Recent Results in the Theory of Graph Spectra*, volume 36 of *Annals of Discrete Mathematics*. North-Holland, 1988.

[CDS79] Dragoš M. Cvetković, Michael Doob, and Horst Sachs. *Spectra of Graphs – Theory and Applications*. Deutscher Verlag der Wissenschaften Berlin, 1979.

[Chu97] Fan R. K. Chung. *Spectral Graph Theory*. Number 92 in Regional Conference Series in Mathematics. American Mathematical Society, 1997.

[Cio11] Sebastian M. Cioabă. Some applications of eigenvalues of graphs. In Matthias Dehmer, editor, *Structural Analysis of Complex Networks*, chapter 14, pages 357–379. Birkhäuser, 2011.

[CR90] Dragoš M. Cvetković and Peter Rowlinson. The largest eigenvalue of a graph: A survey. *Linear and Multilinear Algebra*, 28(1):3–33, October 1990.

[CRS97] Dragoš M. Cvetković, Peter Rowlinson, and Slobodan K. Simić. *Eigenspaces of Graphs*, volume 66 of *Encyclopedia of mathematics and its applications*. Cambridge University Press, 1997.

[CS57] Lothar Collatz and Ulrich Sinogowitz. Spektren endlicher Grafen. *Abhandlungen aus dem Mathematischen Seminar der Universität Hamburg*, 21(1):63–77, December 1957.

[Cve70] Dragoš M. Cvetković. The generating function for variations with restrictions and paths of the graph and self-complementary graphs. *Univ. Beograd, Publ. Elektrotehn. Fak., Ser. Mat. Fiz.*, 320–328(322):27–34, 1970.

[Cve71] Dragoš M. Cvetković. Graphs and their spectra. *Univ. Beograd, Publ. Elektrotehn. Fak., Ser. Mat. Fiz.*, 354–456(354):1–50, 1971.

[Cve09] Dragoš M. Cvetković. Applications of graph spectra: An introduction to the literature. In *Applications of Graph Spectra*, volume 13(21) of *Zbornik radova*, pages 7–31. Mathematical Institute SANU, Belgrade, June 2009.

[CWW+08] Deepayan Chakrabarti, Yang Wang, Chenxi Wang, Jurij Leskovec, and Christos Faloutsos. Epidemic thresholds in real networks. *ACM Transactions on Information and System Security*, 10(4):13:1–13:26, January 2008.

[DG03]   Andreas Dress and Ivan Gutman. The number of walks in a graph. *Applied Mathematics Letters*, 16(5):797–801, July 2003.

[ES82]   Paul Erdős and Miklós Simonovits. Compactness results in extremal graph theory. *Combinatorica*, 2(3):275–288, 1982.

[FKP01]   Uriel Feige, Guy Kortsarz, and David Peleg. The dense k-subgraph problem. *Algorithmica*, 29(3):410–421, December 2001.

[Gut01]   Ivan Gutman. The energy of a graph: Old and new results. In *Proceedings of the Euroconference Algebraic Combinatorics and Applications (ALCOMA'99)*, pages 196–211. Springer, 2001.

[HKM+11]   Raymond Hemmecke, Sven Kosub, Ernst W. Mayr, Hanjo Täubig, and Jeremias Weihmann. Inequalities for the number of walks in trees and general graphs and a generalization of a theorem of Erdős and Simonovits. Technical Report TUM-I1109, Department of Computer Science, Technische Universität München, April 2011.

[HKM+12]   Raymond Hemmecke, Sven Kosub, Ernst W. Mayr, Hanjo Täubig, and Jeremias Weihmann. Inequalities for the number of walks in graphs. In *Proceedings of the 9th Meeting on Analytic Algorithmics and Combinatorics (ANALCO'12)*, pages 26–39. SIAM, 2012.

[Hof70]   Alan J. Hoffman. On eigenvalues and colorings of graphs. In Bernard Harris, editor, *Graph Theory and Its Applications*, pages 79–91. Academic Press, 1970.

[Hof88]   M. Hofmeister. Spectral radius and degree sequence. *Mathematische Nachrichten*, 139(1):37–44, 1988.

[Hof94]   M. Hofmeister. A note on almost regular graphs. *Mathematische Nachrichten*, 166(1):259–262, 1994.

[HS79]   Frank Harary and Allen J. Schwenk. The spectral approach to determining the number of walks in a graph. *Pacific Journal of Mathematics*, 80(2):443–449, 1979.

[HTW07]   Yaoping Hou, Zhen Tang, and Chingwah Woo. On the spectral radius, k-degree and the upper bound of energy in a graph. *MATCH: Communications in Mathematical and in Computer Chemistry*, 57(2):341–350, 2007.

[HZ05]   Yuan Hong and Xiao-Dong Zhang. Sharp upper and lower bounds for largest eigenvalue of the Laplacian matrices of trees. *Discrete Mathematics*, 296(2-3):187–197, July 2005.

[IS09]   Aleksandar Ilić and Dragan Stevanović. On comparing Zagreb indices. *MATCH: Communications in Mathematical and in Computer Chemistry*, 62(3):681–687, 2009.

[Kos05]   Sven Kosub. Local density. In Ulrik Brandes and Thomas Erlebach, editors, *Network Analysis – Methodological Foundations*, volume 3418 of *Lecture Notes in Computer Science*, pages 112–142. Springer, 2005.

[LMSM83]   Jeffrey C. Lagarias, James E. Mazo, Lawrence A. Shepp, and Brendan D. McKay. An inequality for walks in a graph. *SIAM Review*, 25(3):403, July 1983.

[LMSM84]   Jeffrey C. Lagarias, James E. Mazo, Lawrence A. Shepp, and Brendan D. McKay. An inequality for walks in a graph. *SIAM Review*, 26(4):580–582, October 1984.

[Lon66]   David London. Inequalities in quadratic forms. *Duke Mathematical Journal*, 33(3):511–522, September 1966.

[McC71]   B. J. McClelland. Properties of the latent roots of a matrix: The estimation of π-electron energies. *The Journal of Chemical Physics*, 54(2):640–643, January 1971.

[MN62]   Marvin Marcus and Morris Newman. The sum of the elements of the powers of a matrix. *Pacific Journal of Mathematics*, 12(2):627–635, June 1962.

[MS59]   H. P. Mulholland and Cedric A. B. Smith. An inequality arising in genetical theory. *The American Mathematical Monthly*, 66(8):673–683, October 1959.

[MS60]   H. P. Mulholland and Cedric A. B. Smith. Corrections: An inequality arising in genetical theory. *The American Mathematical Monthly*, 67(2):161, February 1960.

[Nik06]   Vladimir Nikiforov. Walks and the spectral radius of graphs. *Linear Algebra and its Applications*, 418(1):257–268, October 2006.

[Nos70]   Eva Nosal. Eigenvalues of graphs. Master's thesis, University of Calgary, 1970.

[VM11]   Piet Van Mieghem. *Graph Spectra for Complex Networks*. Cambridge University Press, 2011.

[Wil86]   Herbert S. Wilf. Spectral bounds for the clique and independence numbers of graphs. *Journal of Combinatorial Theory, Series B*, 40(1):113–117, February 1986.

[YLT04]   Aimei Yu, Mei Lu, and Feng Tian. On the spectral radius of graphs. *Linear Algebra and its Applications*, 387:41–49, August 2004.