Inequalities for the Number of Walks in Graphs

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Abstract

We investigate the growth of the number w_k of walks of length k in undirected graphs as well as related inequalities. In the first part, we derive the inequalities $w_{2a+c} \cdot w_{2(a+b)+c} \leq w_{2a} \cdot w_{2(a+b+c)}$ and $w_{2a+c}(v,v) \cdot w_{2(a+b)+c}(v,v) \leq w_{2a}(v,v) \cdot w_{2(a+b+c)}(v,v)$ for the number $w_k(v,v)$ of closed walks of length k starting at a given vertex v. The first is a direct implication of a matrix inequality by Markus and Newman and generalizes two inequalities by Lagarias et al. and Dress & Gutman. We then use an inequality of Blakley and Dixon to show the inequality $w_{2\ell+p}^k \leq w_{2\ell+pk} \cdot w_{2\ell}^{k-1}$ which also generalizes the inequality by Dress and Gutman and also an inequality by Erdős and Simonovits. Both results can be translated directly into the corresponding forms using the higher order densities, which extends former results.

In the second part, we provide a new family of lower bounds for the largest eigenvalue λ_1 of the adjacency matrix based on closed walks and apply the before mentioned inequalities to show monotonicity in this and a related family of lower bounds of Nikiforov. This leads to generalized upper bounds for the energy of graphs.

In the third part, we demonstrate that a further natural generalization of the inequality $w_{2a+c} \cdot w_{2(a+b)+c} \leq w_{2a} \cdot w_{2(a+b+c)}$ is not valid for general graphs. We show that $w_{a+b} \cdot w_{a+b+c} \leq w_a \cdot w_{a+2b+c}$ does not hold even in very restricted cases like $w_1 \cdot w_2 \leq w_0 \cdot w_3$ (i.e., $\bar{d} \cdot w_2 \leq w_3$) in the context of bipartite or cycle free graphs. In contrast, we show that surprisingly this inequality is always satisfied for trees and show how to construct worst-case instances (regarding the difference of both sides of the inequality) for a given degree sequence. We also provide a proof for the inequality $w_1 \cdot w_4 \leq w_0 \cdot w_5$ (i.e., $\bar{d} \cdot w_4 \leq w_5$) for trees and conclude with a corresponding conjecture for longer walks.

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1 Introduction

1.1 Notation and basic facts Throughout the paper we assume that $\mathbb{N}$ denotes the set of nonnegative integers. 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 One of the reasons to investigate the growth of the number of walks was a paper by Feige, Kortsarz, and Peleg [FKP01] on approximating the Dense k-Subgraph Problem that used the following observation: In a graph with n vertices and average degree $\overline{d}$, there exist two vertices v_i, v_j such that $\overline{d}^k/n \leq w_k(v_i, v_j)$. 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 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. Apparently, they were not aware of the fact, that this inequality had already been conjectured for all k by Erdős and Simonovits (and in fact Godsil, see [ES82]). Godsil noticed that the inequality can be proven using the results of Mulholland and Smith [MS59, MS60], Blakley and Roy [BR65], and London [Lon66]. Quite recently, we came to know that there is also 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 1.1. (ERDŐS & SIMONOVITS) *In undirected graphs holds for all $k \in \mathbb{N}$: $w_1^k \le w_0^{k-1} w_k$.*

Lagarias, Mazo, Shepp, and McKay [LMSM83] posed the question for which numbers r and s the following inequality holds for all graphs: $w_r \cdot w_s \overset{?}{\le} n \cdot w_{r+s}$. 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 1.2. (LAGARIAS ET AL.) *In undirected graphs holds for all $a, b \in \mathbb{N}$: $w_{2a+b} \cdot w_b \le w_0 \cdot w_{2(a+b)}$.*

Furthermore, Lagarias et al. presented counterexamples whenever $r + s$ is odd [LMSM84]. Nevertheless they noted without proof, that for any graph G there is a constant c, s.t. for all $r, s \ge c$ the inequality is valid. This could be very useful in situations where only asymptotic results are necessary.

Dress and Gutman [DG03] reported the following inequality:

THEOREM 1.3. (DRESS & GUTMAN) *In undirected graphs holds for all $a, b \in \mathbb{N}$: $w_{a+b}^2 \le w_{2a} \cdot w_{2b}$.*

For the proof, they applied the Cauchy-Schwarz inequality to the number of walks:
$\left[\sum_{v\in V} w_a(v) w_b(v)\right]^2 \le \left[\sum_{v\in V} w_a(v)^2\right]\left[\sum_{v\in V} w_b(v)^2\right]$.

Regarding the sums of powers of the degrees, Ahlswede and Katona [AK78] investigated the graphs with the maximum number of walks of length 2. Later, de Caen [dC98] provided for $n \ge 2$ the inequality $w_2 = \sum_{v\in V} d_v^2 \le m\left(\frac{2m}{n-1} + n - 2\right)$. Quite recently, Nikiforov [Nik07] showed the following inequality:

$$w_2 \le \begin{cases} (2m)^{3/2} & \text{for } m \ge n^2/4 \\ (n^2-2m)^{3/2} + 4mn - n^3 & \text{for } m < n^2/4 \end{cases}.$$

Fiol and Garriga [FG09] proved that $w_k \le \sum_{x\in V} d_x^k$.

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

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

These results were generalized by Nikiforov [Nik06] to $\frac{w_{k+r}}{w_k} \le \lambda_1^r$ for all $r \ge 1$ and *even* numbers $k \ge 0$.[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: $\frac{w_r}{n} \le \lambda_1^r$ and $\frac{w_{2\ell+1}}{w_{2\ell}} \le \lambda_1$ 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 $r \ge 1$ and $k \ge 0$: $\lambda_1^r \le \max_{v\in V} \frac{w_{k+r}(v)}{w_k(v)}$.

Nosal [Nos70] proved another lower bound for the spectral radius using the square root of the maximum degree: $\sqrt{\Delta} \le \lambda_1$ 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 $1 - \lambda_1/\lambda_n \le \chi(G)$, see [Hof70]), the clique number (using an inequality of Wilf $n/(n - \lambda_1) \le \omega$, 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].

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 ($1 \le i \le n$) 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 $A = UDU^T$ 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. Since U is an orthonormal matrix, we know that its column and row vectors have unit length:

[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.

$$\forall x: \sum_{i=1}^{n} u_{xi}^2 = 1 \quad \text{as well as} \quad \forall y: \sum_{i=1}^{n} u_{iy}^2 = 1$$

and they are pairwise orthogonal, i.e., for $x \neq y$:

$$\sum_{i=1}^{n} u_{xi} u_{yi} = 0 \quad \text{as well as} \quad \sum_{i=1}^{n} u_{ix} u_{iy} = 0.$$

The number of walks of length k from vertex i to vertex j is exactly the (i,j)-entry of the matrix power $A^k = (UDU^T)^k = UD^kU^T$. The total number of walks of length k is $w_k = \langle \mathbf{1}_n, A^k \mathbf{1}_n \rangle = \left\langle \mathbf{1}_n, \left(UDU^T\right)^k \mathbf{1}_n \right\rangle = \left\langle \mathbf{1}_n, \left(UD^kU^T\right) \mathbf{1}_n \right\rangle$, 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

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

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 $U^TAU = D = \mathrm{diag}(\lambda_1 \ldots \lambda_n)$ 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 $U^TA^kU = (U^TAU)^k = D^k = \mathrm{diag}(\lambda_1^k \ldots \lambda_n^k)$: $\lambda_i^k = \sum_{x\in V, y\in V} w_k(x,y) u_{xi} u_{yi}$. 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 $U^TAU = U^{-1}AU = D$, 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 Generalized inequalities for the number of walks of length k and the kth-order densities

2.1 A unifying generalization of the inequalities of Lagarias et al. and Dress & Gutman

Theorem 1.2 (the inequality of Lagarias et al.) and Theorem 1.3 (the inequality of Dress and Gutman) are special cases of the following inequality:

Theorem 2.1. (Sandwich Theorem) *For all integers $a, b, c \in \mathbb{N}$ and all nodes $v \in V$ holds:*

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

and

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

Actually, the theorem does not only hold for adjacency matrices. It can be extended to Hermitian matrices. While the entries are then complex numbers, the sum of all entries as well as the entries on the main diagonal are all real. The proof is very similar for both parts of the theorem. It is based on the observation that the difference of both sides of the inequality can be written as a sum of nonnegative terms.

In this subsection we assume the more general case where A is a Hermitian matrix. Then the sum of all entries is a real number, as well as each entry on the main diagonal. The same applies for 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. We define $B_i = \sum_{x=1}^{n} u_{xi}$ as an abbreviation for the column sums of U. We know that $A^k = (UDU^*)^k = UD^kU^*$. Now the analog for $w_k(x,y)$ is the following: $A^k_{(x,y)} = \sum_{i=1}^{n} u_{xi} \bar{u}_{yi} \lambda_i^k$. The entries on the main diagonal are $A^k_{(x,x)} = \sum_{i=1}^{n} u_{xi} \bar{u}_{xi} \lambda_i^k$. The analog of $w_k(x)$ is the sum of entries in row x:

$$\begin{aligned} w_k(x) \quad &= \quad \sum_{y=1}^{n} \sum_{i=1}^{n} u_{xi} \bar{u}_{yi} \lambda_i^k = \sum_{i=1}^{n} \left(u_{xi} \lambda_i^k \sum_{y=1}^{n} \bar{u}_{yi} \right) \\ &= \quad \sum_{i=1}^{n} u_{xi} \bar{B}_i \lambda_i^k \end{aligned}$$

Then, the total sum of the entries is

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

Now consider the following term with nonnegative coefficients p_i:

$$\begin{aligned}
&\sum_{i=1}^{n} p_i \lambda_i^{2a} \sum_{j=1}^{n} p_j \lambda_j^{2(a+b+c)} \\
&- \sum_{i=1}^{n} p_i \lambda_i^{2a+c} \sum_{j=1}^{n} p_j \lambda_j^{2a+2b+c} \\
= &\sum_{i=1}^{n} \sum_{j=1}^{n} p_i p_j \left(\lambda_i^{2a} \lambda_j^{2(a+b+c)} - \lambda_i^{2a+c} \lambda_j^{2a+2b+c} \right) \\
= &\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} p_i p_j \Big(\lambda_i^{2a} \lambda_j^{2(a+b+c)} - \lambda_i^{2a+c} \lambda_j^{2a+2b+c} \\
&\qquad + \lambda_j^{2a} \lambda_i^{2(a+b+c)} - \lambda_j^{2a+c} \lambda_i^{2a+2b+c} \Big) \\
= &\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} p_i p_j \lambda_i^{2a} \lambda_j^{2a} \Big(\lambda_j^{2(b+c)} - \lambda_i^{c} \lambda_j^{2b+c} \\
&\qquad + \lambda_i^{2(b+c)} - \lambda_j^{c} \lambda_i^{2b+c} \Big) \\
= &\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} p_i p_j \lambda_i^{2a} \lambda_j^{2a} \left(\lambda_j^{2b+c} - \lambda_i^{2b+c} \right) \left(\lambda_j^{c} - \lambda_i^{c} \right)
\end{aligned}$$

Each term within the last line must be nonnegative, since $p_i p_j \lambda_i^{2a} \lambda_j^{2a}$ is nonnegative, and $(\lambda_j^{2b+c} - \lambda_i^{2b+c})$ and $(\lambda_j^{c} - \lambda_i^{c})$ must have the same sign.

Note that the product of a complex number and its conjugate is a nonnegative real number. Thus, by setting $p_i = B_i \bar{B}_i$ we get the sandwich theorem for the total sum of the matrix entries:

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

Setting $p_i = u_{v,i} \bar{u}_{v,i}$ yields the statement for the entries on the main diagonal:

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

Note that the first part of the statement had already been obtained by Marcus and Newman [MN62].

The density implication: 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 $\rho_1 = \rho$).

Theorem 2.1 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 2.1. *For all $a, b, c \in \mathbb{N}$ holds:*

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

2.2 A unifying generalization of the inequalities of Erdős & Simonovits and Dress & Gutman We now show a generalization of Theorem 1.1 (the inequality of Erdős and Simonovits) which is at the same time another generalization of Theorem 1.3 (the inequality of Dress and Gutman). While our first proof in [HKM+11] used a theorem of Blakley and Roy [BR65], we now give an even more direct proof by using the following theorem:

Theorem 2.2. (Blakley & Dixon [BD66]) *For any positive integer q, nonnegative real n-vector u and nonnegative real symmetric $n \times n$-matrix S holds:*

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

The number of walks of length k can be counted in the following way: $w_k = \langle \mathbf{1}_n, A^k \mathbf{1}_n \rangle$. The same method can be applied if we replace the $\mathbf{1}_n$ vector by the vector $\vec{w}_\ell$ of walks of length ℓ that start at each vertex. This way, each of the length-k walks from vertex x to vertex y is multiplied by $w_\ell(x)$ and $w_\ell(y)$, i.e., the number of length-ℓ walks starting at x and y, 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 $k + 2\ell$. Now, the application of Theorem 2.2 to the matrix $S = A^p$ and the vector $u = \vec{w}_\ell$, and setting $q = k - 1$ (note that for $\langle u, u \rangle \neq 0$ and $q \in \{-1, 0\}$ both sides are equal) yields the following statement:

Theorem 2.3. *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 $w_{2\ell} > 0$ (in particular for graphs having at least one edge), this is equivalent to

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

Setting $k = 2$ leads to $w_{2\ell+p}^{2} \leq w_{2\ell+2p} \cdot w_{2\ell}$ and therefore results in Theorem 1.3 published by Dress and Gutman. On the other hand, 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 2.2. *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 1.1 reported by Erdős and Simonovits.

A similar result can be shown for the number of closed walks starting at a given vertex v. We only need the following observations regarding the vector $\vec{w}_\ell(v)$ of the number of walks from vertex v to all other vertices: $\vec{w}_\ell(v)^T \vec{w}_\ell(v) = w_{2\ell}(v,v)$ and $\vec{w}_\ell(v)^T A^k \vec{w}_\ell(v) = w_{2\ell+k}(v,v)$.

Again, the application of Theorem 2.2 yields similar as above:

Theorem 2.4. *For all graphs, the following inequality regarding the number of closed walks is valid for each vertex v and for $k, \ell, p \in \mathbb{N}$ 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

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

The density implication: Theorem 2.3 implies

$$\frac{w_{2\ell+p}^k}{[n(n-1)^{2\ell+p}]^k} \leq \frac{w_{2\ell+pk} \cdot w_{2\ell}^{k-1}}{n(n-1)^{2\ell+pk} \cdot [n(n-1)^{2\ell}]^{k-1}}$$

Corollary 2.3. *For all graphs and $k, \ell, p \in \mathbb{N}$, the following inequality holds: $\rho_{2\ell+p}^k \leq \rho_{2\ell+pk} \cdot \rho_{2\ell}$.*

This extends the known relations (see [Kos05]) and includes as special cases: $\rho_p^k \leq \rho_{pk}$ $(\ell = 0)$ and $\rho^k \leq \rho_k$ $(\ell = 0, p = 1)$.

3 Generalized bounds for the spectral radius and the graph energy

3.1 Lower bound for the spectral radius We now show a generalization of the lower bound $\sqrt{\Delta} \leq \lambda_1$ for the largest eigenvalue that was shown by Nosal [Nos70]. For every principal submatrix A' of the adjacency matrix A we know that $\lambda(A) \geq \lambda(A')$ where $\lambda(M)$ denotes the largest eigenvalue of matrix M. In particular, we can apply this inequality to each entry of the main diagonal: $\lambda(A) \geq A_{i,i}$. Thus, we know that $\lambda(A) = \sqrt[k]{\lambda(A^k)} \geq \sqrt[k]{(A^k)_{i,i}} = \sqrt[k]{w_k(v_i,v_i)}$ for each $v_i \in V$. We can rewrite this in the following way: The largest eigenvalue λ_1 of the adjacency matrix is bounded from below by the k-th root of the number of *closed* walks of length k:

$$\lambda_1 \geq \max_{v \in V} \sqrt[k]{w_k(v,v)}$$

The special case $\ell = 2$ corresponds to the bound of Nosal (since $w_2(v,v) = d_v$).

The application of the Rayleigh-Ritz Theorem leads to an even more general lower bound for the spectral radius of graphs. The theorem states that for a Hermitian matrix $A \in \mathbb{C}^{n \times n}$ the eigenvectors are the critical points (vectors) of the Rayleigh quotient, which is the real function

$$R(\mathbf{x}) = \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \qquad ||\mathbf{x}|| \neq 0$$

and its eigenvalues are its values at such critical points. In particular, we know $\lambda_1 = \max_{||\mathbf{x}|| \neq 0} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$. We conclude for a vertex $v \in V$ with $w_\ell(v) > 0$:

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

Theorem 3.1. *For arbitrary graphs, the spectral radius of the adjacency matrix satisfies the following inequality:*

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

The case $\ell = 0$ 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 by Nosal.

3.2 Monotonicity 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. The same is shown for Nikiforov's lower bound. Correspondingly, we define two families of lower bounds in case $w_{2\ell}(v,v) > 0$ and $w_{2\ell} > 0$:

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

Lemma 3.1. *For $k, \ell, x, y \in \mathbb{N}$ with $k \geq 1$ holds*

$$\max_{v \in V} F_{k+x,\ell+y}(v) \quad \geq \quad \max_{v \in V} F_{k,\ell}(v) \qquad \textit{and}$$
$$G_{k+x,\ell+y} \quad \geq \quad G_{k,\ell}$$

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

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

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

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

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

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

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

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

A proof for the second part of the lemma ($G_{k+x,\ell+y} \geq G_{k,\ell}$) results from replacing each occurrence of $w_i(v,v)$ by w_i in the proof above.

Theorems 2.4 and 2.3 directly imply additional monotonicity results for our new bound, as well as for Nikiforov's bound:

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

In contrast to Lemma 3.1, 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

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

which implies $f(\lambda_1) \leq f(G_{k,\ell})$ 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

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

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

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

4 Counterexamples for special cases

Since Lagarias et al. [LMSM84] disproved the inequality $w_r \cdot w_s \leq n \cdot w_{r+s}$ for odd values of the sum $r+s$ it would be interesting to prove or disprove validity for more restricted graph classes, such as the class of all bipartite graphs, the class of all cycle-free graphs (forests), and the class of all trees.

4.1 Bipartite graphs We show that bipartite graphs violate the inequality $w_r \cdot w_s \leq n \cdot w_{r+s}$, in particular for $r = 2$, $s = 1$. Similar to the general counterexamples proposed in [LMSM84], our counterexamples consist of two parts: a star and (instead of complete graphs) complete bipartite graphs. Consider for instance the graph consisting of the complete bipartite graph $B_{2,2}$ and the star S_6. For this graph, we have $w_0 = 4 + 6$, $w_1 = 8 + 10$, $w_2 = 16 + 30$, and $w_3 = 32 + 50$. Hence, the inequality is violated: $w_1 w_2 = 828 \not\leq 820 = w_0 w_3$. This way we found an even smaller (disconnected) counterexample. Connected counterexamples can be constructed by appropriate scaling and attaching both parts through a single edge (q.v. [LMSM84]).

4.2 Forests We now show, that there are arbitrarily large cycle-free graphs (forests) that contradict the inequality. These graphs, again, consist of two parts. This time, the two compounds of the graph are a path and a star. The respective number of walks are (for the path assume $n \geq 3$):

$$\begin{array}{ll}
w_0(P_n) = n & = n \\
w_1(P_n) = 2(n-1) & = 2n-2 \\
w_2(P_n) = (n-2)\cdot 2^2 + 2\cdot 1^2 & = 4n-6 \ (n \geq 2) \\
w_3(P_n) = 2[(n-3)\cdot 2\cdot 2 + 2\cdot 2\cdot 1] & = 8n-16 \ (n \geq 3) \\
\hline
w_0(S_n) = n & \\
w_1(S_n) = 2(n-1) & \\
w_2(S_n) = n(n-1) & \\
w_3(S_n) = 2(n-1)^2 &
\end{array}$$

Now consider a graph consisting of a star S_x and a path P_y. Then the inequality reads as follows:

$$(x+y)(2\cdot(x-1)^2 + 8y - 16) \geq$$
$$(x(x-1) + 4y - 6)(2(x-1) + 2(y-1))$$
$$x^2 - 3x - xy + 7y - 12 \geq 0$$

Values for x from 2 to 7 lead to inequalities that are true for $y > 2$, but already $x = 8$ leads to $-y + 28 \geq 0$ which does not hold for $y \geq 29$. Thus, a possible counterexample consists of star S_8 and path P_{29}. Most surprisingly, the connected variant is no longer a counterexample as we will see later.

4.3 Construction of worst case trees In order to answer the question whether the inequality $w_1 w_2 \leq w_0 w_3$ holds for all trees we investigate the behavior of different trees with respect to the value of the difference of both sides, i.e. $w_0 w_3 - w_1 w_2$. Within this subsection, we will show how to construct trees of a given degree sequence that minimize this difference (i.e., "worst case trees"). Later on, our aim is to show that certain graph transformations change the value of the difference in a certain direction which leads to a proof of the inequality.

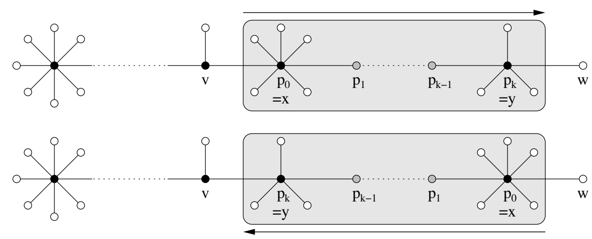

Figure 1: Path inversion in a (caterpillar) tree

LEMMA 4.1. *For a given degree sequence of a tree, the tree that minimizes the value of the difference $w_0 w_3 - w_1 w_2$ cannot have four different vertices $v, w, x, y \in V$ with $d_x > d_y$ and $d_v > d_w$ such that x and y are the neighbors of v and w (resp.) on the path from v to w.*

Proof. Assume the contrary, i.e., there is a worst case tree (having minimum difference value) for a given degree sequence that has such vertices $v, w, x, y \in V$ (see Figure 1).

Consider the tree that is constructed by inverting the x-y-path between v and w (i.e. x is now connected to the former neighbor w of y, whereas y's connection to w is replaced by the connection to the former neighbor v of x). This tree has the same degree sequence as before, i.e., besides the number of nodes n and the number of edges $m = w_1/2$ also the number of length-2-paths $w_2 = \sum_{v\in V} d_v^2$ has not changed. For the number of length-3-paths $w_3 = 2\sum_{\{s,t\}\in E} d_s d_t$ only the values for the edges connecting the x-y-path to v and w have changed from $d_x d_v + d_y d_w$ to $d_y d_v + d_x d_w$.

$$\begin{array}{rcl}
d_x d_v + d_y d_w & > & d_y d_v + d_x d_w \\
(d_x - d_y)d_v - (d_x - d_y)d_w & > & 0 \\
(d_x - d_y)(d_v - d_w) & > & 0
\end{array}$$

Since $d_x > d_y$ and $d_v > d_w$, the value of w_3 must have become smaller, a contradiction to the assumption that $w_0 w_3 - w_1 w_2$ was a minimum.

At first, we have a look at a special class of trees, namely the caterpillar trees. A caterpillar [tree] is a tree that has all its leaves attached to a central path. For a given degree sequence of a caterpillar, a caterpillar that minimizes the value of the difference $w_0 w_3 - w_2 w_1$ has a vertex of maximum degree as one of the end vertices of its central path. This is a direct consequence of the lemma. Furthermore, the other end vertex of the central path must be the second vertex in the order of non-increasing degrees. (Note that there may be more than one caterpillar tree topology minimizing the difference value in the case where a vertex degree > 1 occurs more than just once.) The next two vertices towards the inside of the central path must be two of the remaining vertices with lowest possible degree.

The lemma directly implies an algorithm for the construction of a worst-case caterpillar (i.e., a caterpillar that minimizes $w_0w_3 - w_2w_1$): From the given degree sequence, we start with the two leaf-ends of the central path (with minimum degree 1) and fill in the remaining vertices from the outside to the middle by alternately considering two remaining vertices of maximum or minimum degree, starting with the two vertices of maximum degree, followed by the two remaining vertices of minimum degree and so on. The only thing that has to be taken care of is that, if the two vertices inserted in the last iteration differ in their degree and also the two vertices to be inserted in the current iteration differ in their degree, then the higher-degree-vertex of one pair must get the edge to the lower-degree-vertex of the other pair and vice versa. The result is a caterpillar that has its vertices of most extreme degrees at the ends of the central path, minimum and maximum alternating towards the center, and the vertices corresponding to the median of the degree sequence are located in the center.

We now consider arbitrary trees. The lemma implies that in a worst-case tree for a given degree sequence, a vertex of maximum degree x cannot have more than one neighboring inner node while at the same time there exists a vertex y with lower degree that has a neighboring leaf w. (Otherwise there is a non-leaf neighbor v of x that is not on the path from x to y and the lemma could be applied since $d_v \geq 2 > d_w = 1$ and $d_x > d_y$.) The lemma not only implies that the vertices of maximum degrees must have as many neighboring leaves as possible, it also implies as a next step that if there is a non-leaf (inner) neighbor of such a vertex, this vertex must have smallest possible degree. Hence we can build a worst-case tree from a given degree sequence from the outside to the inside. The outer shell is the set of leaves, the next layers towards the inside of the tree are made of vertices having largest and smallest possible degree in an alternating fashion. Only one of the valences has to be left for attaching this subtree to the rest of the graph. (Note that there may be several worst-case trees with different topologies if there are vertices having the same degree.)

5 Inequalities for trees

5.1 Stars and paths

Lemma 5.1. *For each star S_n with n vertices the following inequality is valid:* $w_k \cdot w_\ell \leq w_0 \cdot w_{k+\ell}$

Proof. In a star, we observe $w_{2k} = n(n-1)^k$ and $w_{2k+1} = 2(n-1)^{k+1}$.

If $k+\ell$ is odd, then one of the two lengths is odd and the other one is even. W.l.o.g. assume k is odd and ℓ is even. Hence, we get $2(n-1)^{(k-1)/2+1} \cdot n(n-1)^{\ell/2} = n \cdot 2(n-1)^{(k+\ell-1)/2+1}$ with equality of both sides.

In the next case, both of k and ℓ are even. Then we get $n(n-1)^{k/2} \cdot n(n-1)^{\ell/2} = n \cdot n(n-1)^{(k+\ell)/2}$.

But if both of k and ℓ are odd numbers, we obtain $2(n-1)^{(k-1)/2+1} \cdot 2(n-1)^{(\ell-1)/2+1} = 4(n-1)^{(k+\ell)/2+1} \leq n \cdot n(n-1)^{(k+\ell)/2}$ which is a valid inequality because $4(n-1) \leq n^2$.

Note that this inequality can be generalized in the following way: assuming that among the parameters $a, b, c \in \mathbb{N}$ is at least one even number, then we have $w_{a+b} \cdot w_{a+c} \leq w_a \cdot w_{a+b+c}$. By contrast, if all parameters a, b, c are odd numbers, the relation of the inequality is *inverted*. Accordingly, this kind of sandwich theorem cannot be valid in full generality even for trees, since for stars we have $w_2 \cdot w_2 \not\leq w_1 \cdot w_3$ (or $\frac{w_3}{w_2} \not\geq \frac{w_2}{w_1}$), etc.

Lemma 5.2. *For each path P_n with n vertices the following inequality is valid:* $w_1 \cdot w_k \leq w_0 \cdot w_{k+1}$

Proof. Let $P = (V, E)$ be a path with $n \geq 1$ vertices and let b denote a leaf of P and $k \in \mathbb{N}$. Then

$$\begin{aligned} & [nw_{k+1} - 2(n-1)w_k]/n \\ = \quad & w_{k+1} - 2w_k + 2w_k/n \\ = \quad & \sum_{v \in V} d_v w_k(v) - 2 \sum_{v \in V} w_k(v) + 2w_k/n \\ = \quad & \sum_{v \in V} (d_v - 2) w_k(v) + 2w_k/n \\ = \quad & -2w_k(b) + 2w_k/n \end{aligned}$$

Now we show $w_k/n - w_k(b) \geq 0$ by proving $w_k(v) \geq w_k(b)$ for every vertex v.

Case 1: The distance between v and b is even. For each walk starting at b, we construct a unique walk starting at v by symmetrically mimicking all moves until both walks meet at the same vertex. After that, the new walk uses the same edges as the walk that started at b.

Case 2: The distance between v and b is odd. If v is the other leaf, then because of symmetry we are done. Thus, assume that v is not a leaf. Now, we construct the corresponding walk in much the same way as in the first case, but we ignore the first move which is fixed anyways. Now the distance to v is even and we apply the same method as in the first case (which is possible since v is not a leaf). After that, the last move can be chosen arbitrarily.

5.2 The w_3-inequality for trees Let $w_{i,j}$ and $w_{i,j}(v)$ denote the number of walks (total or starting at $v \in V$, resp.) having length i, where the last j steps constitute a *path*, i.e., a vertex-disjoint walk of length j.

FACT 5.1. *For each vertex $v \in V$ and all $i \in \mathbb{N} \setminus \{0\}$ holds $w_{i+1}(v) = w_{i+1,2}(v) + w_i(v)$. Obviously, this implies $w_{i+1} = w_{i+1,2} + w_i$.*

THEOREM 5.1. *For all trees the following inequality is valid: $w_1 \cdot w_2 \leq w_0 \cdot w_3$.*

Proof. Besides $w_0 = n$, we know (for trees):

$$\begin{aligned} w_1 &= 2(n-1) \\ w_2 &= w_{2,2} + w_1 = p_2 + w_1 \\ w_3 &= w_{3,2} + w_2 = p_3 + p_2 + w_2 = p_3 + 2p_2 + w_1 \end{aligned}$$

Consider the difference of both sides of the inequality:

$$\begin{aligned} w_0 w_3 - w_1 w_2 &= n w_3 - 2(n-1) w_2 \\ &= n(w_3 - 2w_2) + 2w_2 \\ &= n[p_3 - 2n + 6] + 2(p_2 - 2) \end{aligned}$$

Note that each tree with diameter at most 2 is a star. In this case we have $w_0 w_3 = w_1 w_2$ (see Lemma 5.1).

Let $G = (V, E)$ be any tree that satisfies the conditions $\text{diam}(G) \geq 3$, $(p_3 - 2n + 6) \geq 0$ and $w_0 w_3 \geq w_1 w_2$. Then we can create a new tree G' by appending a leaf to any vertex. For G' holds $n' = n+1$, $p'_2 \geq p_2+2$, and $p'_3 \geq p_3+2$. Hence, G' satisfies the three conditions, too.

Each tree having diameter at least 3 can be constructed by repeatedly appending new leaves to a path of length 3. For the path of length 3 we have $n = 4$, $p_2 = 4$, and $p_3 = 2$. Hence, all conditions are fulfilled and therefore all trees observe the above inequality.

5.3 The w_5-inequality for trees

THEOREM 5.2. *For all trees the following inequality is valid: $w_1 \cdot w_4 \leq w_0 \cdot w_5$.*

The proof is a detailed distinction of cases and can be found in Appendix A.

5.4 A conjecture for trees The justification of the inequalities $w_1 w_2 \leq w_0 w_3$ and $w_1 w_4 \leq w_0 w_5$ for trees raise hope for a proof of a more general conjecture by Täubig:

CONJECTURE 5.1. *For all trees the following inequality is valid for all $k \in \mathbb{N}$:*

$$w_1 \cdot w_k \leq w_0 \cdot w_{k+1} \quad \textit{or equivalently} \quad \overline{d} \cdot w_k \leq w_{k+1}$$

(since $w_0 = n$ and $w_1 = 2m$).

Then, in contrast to general graphs, trees would also observe the inequality for all odd (not only even) indices on the greater side. This case of an *odd* index on the greater side is equivalent to a statement about averages: $\frac{1}{n} \sum_{x \in V} w_k(x)^2 \leq \frac{1}{m} \sum_{\{x,y\} \in E} w_k(x) \cdot w_k(y)$.

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A Appendix: Proof for Theorem 5.2 (inequality $w_1 \cdot w_4 \leq w_0 \cdot w_5$ for trees)

Let $G = (V, E)$ be a tree. Then for each $i \in \mathbb{N}$, the following inequalities are equivalent:

$$\begin{aligned} & w_0 w_{i+1} \geq w_1 w_i \\ \Leftrightarrow \quad & n w_{i+1} \geq 2(n-1) w_i \\ \Leftrightarrow \quad & 2w_i + n \sum_{v \in V} d_v w_i(v) - 2n \sum_{v \in V} w_i(v) \geq 0 \\ \Leftrightarrow \quad & 2w_i/n + \sum_{v \in V} (d_v - 2) w_i(v) \geq 0 \end{aligned}$$

Thus, for a proof of the inequality, every i-walk that starts at a leaf creates a negative unit that has to be compensated for by the contribution of the respective neighbors and the correction term $2w_i/n$.

Let b be a leaf attached at an inner vertex x. Then, for $i > 0$, we have $w_i(x) = w_{i+1}(b)$ and by Fact 5.1: $(d_x - 2)w_{i+1}(x) = (d_x - 2)(w_i(x) + w_{i+1,2}(x)) \geq (d_x - 2)w_{i+1}(b)$. So we can use the positive units of an inner node x to compensate for the negative units of at least $d_x - 2$ attached leaves. This is called deficit adjustment at node x.

A.1 Trees with diameter 3 (barbell graphs)

Definition A.1. *An (ℓ, n_1, n_2)-barbell graph is a graph that consists of a path of length ℓ, having attached $n_1 \geq 1$ and $n_2 \geq n_1$ leaves at the two end vertices x_1 and x_2, respectively.*

Each $(1, n_1, n_2)$-barbell graph is a tree having diameter 3 and every tree with diameter 3 is a $(1, n_1, n_2)$-barbell graph for properly chosen n_1, n_2. In the following, we show that for each $i \in \mathbb{N}$ and for every $(1, n_1, n_2)$-barbell graph $G = (V, E)$ (and thus for all trees having diameter 3) holds $w_0 w_{i+1} \geq w_1 w_i$.

Lemma A.1. *For each $(1, n_1, n_2)$-barbell graph and every $i \in \mathbb{N}$ holds $w_i(x_1) \leq w_i(x_2)$.*

Proof. Let b_1 and b_2 be leaves attached to x_1 and x_2, resp. We will show the following equivalent inequalities:

$$\begin{aligned} w_i(x_1) &\leq w_i(x_2) \\ w_{i-1}(x_2) + n_1 w_{i-1}(b_1) &\leq w_{i-1}(x_2) + w_{i,2}(x_2) \end{aligned}$$

For even numbers $i \in 2\mathbb{N}$ this results in:

$$\begin{aligned} & w_{i-1}(x_2) + n_1 w_{i-2}(x_1) \leq \\ & \qquad w_{i-1}(x_2) + n_1 \left[w_{i-2}(x_2) + n_1 w_{i-2}(b_1) \right] \end{aligned}$$

and for odd $i \in 2\mathbb{N} + 1$ this will lead to:

$$w_{i-1}(x_2) + n_1 w_{i-2}(x_1) \leq w_{i-1}(x_2) + n_2 w_{i-2}(x_2)$$

Assume that i is an *even* number. For $i = 0$ we get $w_0(x_1) = 1 = w_0(x_2)$. For the induction, assume that the lemma is valid for all even numbers $i' < i$. Since $w_i(x_2) = w_{i-1}(x_2) + w_{i,2}(x_2)$ (Fact 5.1), it is to show that

$$n_1 w_{i-2}(x_1) \leq w_{i,2}(x_2).$$

Since i is even, the walks of length $i - 2$ starting at x_2 can only end at x_2 or at a leaf attached to x_1. Each of them can be extended by n_1 different paths of length 2, thus $w_{i,2}(x_2) = n_1(w_{i-2}(x_2) + n_1 w_{i-2}(b_1))$.

$$n_1 w_{i-2}(x_1) \leq n_1(w_{i-2}(x_2) + n_1 w_{i-2}(b_1))$$

The proof follows now from the induction hypothesis, i.e., $w_{i-2}(x_1) \leq w_{i-2}(x_2)$.

Assume now, that i is an *odd* number. For $i = 1$ the lemma is true, since $n_1 \leq n_2$. Let $i \geq 3$. Assuming the lemma is valid for all odd numbers $i' < i$, the inequality follows from $n_1 \leq n_2$, the induction hypothesis $w_{i-2}(x_1) \leq w_{i-2}(x_2)$ and the following consideration: each walk of length $i - 2$ starting at x_2 ends at x_1 or a leaf of x_2 and each of those walks can be extended by exactly n_2 paths of length 2.

Lemma A.2. *For each $(1, n_1, n_2)$-barbell graph and every $i \in \mathbb{N}$ holds $n w_{i+1} \geq 2(n-1) w_i$.*

Proof. For $i = 0$ both sides are equal, thus assume $i > 0$. Let b_1 and b_2 be leaves attached to x_1 and x_2, resp. We perform a deficit adjustment at the nodes x_1 and x_2. There are $(d_{x_1} - 1)$ and $(d_{x_2} - 1)$ leaves attached at x_1 and x_2. $(d_{x_1} - 2)$ and $(d_{x_2} - 2)$ of them can be compensated for by the excess terms of x_1 and x_2. Hence, at most $w_i(b_1) + w_i(b_2) = w_{i-1}(x_1) + w_{i-1}(x_2)$ negative units remain unbalanced.

Now we show $2w_i/n \geq w_{i-1}(x_1) + w_{i-1}(x_2)$. By Fact 5.1, we know that $w_{i-1}(x_1) \leq w_i(x_1)$ and $w_{i-1}(x_2) \leq w_i(x_2)$. Lemma A.1 implies $w_{i-1}(x_1) \leq w_{i-1}(x_2)$, and since $n_1 \leq n_2$ we get: $n_1 w_{i-1}(x_1) + n_2 w_{i-1}(x_2) \geq n_1 w_{i-1}(x_2) + n_2 w_{i-1}(x_1)$.

$$\begin{aligned} & 2w_i/n \\ = \; & 2[n_1 w_i(b_1) + w_i(x_1) + n_2 w_i(b_2) + w_i(x_2)]/n \\ = \; & 2[n_1 w_{i-1}(x_1) + w_i(x_1) \\ & + n_2 w_{i-1}(x_2) + w_i(x_2)]/n \\ \geq \; & [n_1 w_{i-1}(x_1) + n_2 w_{i-1}(x_1) + 2w_i(x_1) \\ & + n_1 w_{i-1}(x_2) + n_2 w_{i-1}(x_2) + 2w_i(x_2)]/n \\ \geq \; & [n_1 w_{i-1}(x_1) + n_2 w_{i-1}(x_1) + 2w_{i-1}(x_1) \\ & + n_1 w_{i-1}(x_2) + n_2 w_{i-1}(x_2) + 2w_{i-1}(x_2)]/n \\ \geq \; & \left[n w_{i-1}(x_1) + n w_{i-1}(x_2) \right]/n \\ = \; & w_{i-1}(x_1) + w_{i-1}(x_2) \end{aligned}$$

A.2 $(2, n_1, n_2)$-barbell graphs

Lemma A.3. *For each $(2, n_1, n_2)$-barbell graph holds $w_i(x_1) \leq w_i(x_2)$.*

Proof. For each walk starting at x_1, we can construct a unique walk of the same length that starts at x_2: Since $n_1 \leq n_2$, we can injectively map each leaf of x_1 to a leaf of x_2. For each walk starting at x_1, we mimic this walk (using the mapping) until the walk passes the center. From this point on, we follow exactly the same way (without using the mapping).

Lemma A.4. *For each $(2, n_1, n_2)$-barbell graph and every $i \in \mathbb{N}$ holds $nw_{i+1} \geq 2(n-1)w_i$.*

Proof. Let b_1 and b_2 be leaves attached to x_1 and x_2, resp. We perform a deficit adjustment at the nodes x_1 and x_2. Hence, at most $w_i(b_1) + w_i(b_2) = w_{i-1}(x_1) + w_{i-1}(x_2)$ negative units remain unbalanced.

Now, we show $2w_i/n \geq w_{i-1}(x_1) + w_{i-1}(x_2)$. By Fact 5.1, we know that $w_{i-1}(x_1) \leq w_i(x_1)$ and $w_{i-1}(x_2) \leq w_i(x_2)$. Furthermore, the graph center c fulfills the equality $w_i(c) = w_{i-1}(x_1) + w_{i-1}(x_2)$. Now, from $n_1 \leq n_2$ and Lemma A.3 we obtain:

$$\begin{aligned}
& 2w_i/n \\
= {} & 2[n_1 w_i(b_1) + w_i(x_1) + n_2 w_i(b_2) + w_i(x_2) + w_i(c)]/n \\
= {} & 2[n_1 w_{i-1}(x_1) + w_i(x_1) + w_{i-1}(x_1) + n_2 w_{i-1}(x_2) + w_i(x_2) + w_{i-1}(x_2)]/n \\
= {} & 2[(n_1+1)w_{i-1}(x_1) + w_{i-1}(x_1) + w_{i,2}(x_1) + (n_2+1)w_{i-1}(x_2) + w_{i-1}(x_2) + w_{i,2}(x_2)]/n \\
= {} & 2[(n_1+2)w_{i-1}(x_1) + w_{i,2}(x_1) + (n_2+2)w_{i-1}(x_2) + w_{i,2}(x_2)]/n \\
\geq {} & [(n_1+n_2+4)w_{i-1}(x_1) + 2w_{i,2}(x_1) + (n_1+n_2+4)w_{i-1}(x_2) + 2w_{i,2}(x_2)]/n \\
\geq {} & [(n_1+n_2+3)w_{i-1}(x_1) + (n_1+n_2+3)w_{i-1}(x_2)]/n \\
\geq {} & [nw_{i-1}(x_1) + nw_{i-1}(x_2)]/n \\
\geq {} & w_{i-1}(x_1) + w_{i-1}(x_2)
\end{aligned}$$

A.3 Proof for the w_5-inequality for trees

Proof. To simplify matters, we denote by $N_i(v)$ both, the set as well as the number of nodes having distance i from v. Further, let p_i denote the number of directed paths (i.e., vertex-disjoint walks) of length i. Besides $w_1(v) = d_v$, $w_2(v) = d_v + N_2(v)$, and $w_3(v) = d_v^2 + N_2(v) + N_3(v)$ we observe the following equalities for trees:

$$\sum_{v \in V} (d_v - 1)N_i(v) = \sum_{v \in V} N_{i+1}(v) = p_{i+1}$$

$$\sum_{v \in V} d_v N_i(v) = p_i + p_{i+1}$$

$$\sum_{v \in V} N_2(v)^2 = p_2 + p_4 + \sum_{v \in V} d_v(d_v-1)(d_v-2)$$

$$\sum_{v \in V} N_2(v)N_3(v) = p_3 + p_5 + \sum_{v \in V} N_2(v)(d_v-1)(d_v-2)$$

$$\begin{aligned}
w_4 &= \sum_{v \in V} w_2(v)^2 = \sum_{v \in V} [d_v + N_2(v)]^2 \\
&= \sum_{v \in V} d_v^2 + 2d_v N_2(v) + N_2(v)^2 \\
&= w_2 + 3p_2 + 2p_3 + p_4 + \sum_{v \in V} d_v(d_v-1)(d_v-2)
\end{aligned}$$

$$\begin{aligned}
w_4 &= \sum_{v \in V} w_1(v) w_3(v) = \sum_{v \in V} d_v \cdot [d_v^2 + N_2(v) + N_3(v)] \\
&= \left[\sum_{v \in V} d_v^3\right] + p_2 + 2p_3 + p_4
\end{aligned}$$

$$\begin{aligned}
w_5 &= \sum_{v \in V} w_2(v) w_3(v) \\
&= \sum_{v \in V} [d_v + N_2(v)] \cdot [d_v^2 + N_2(v) + N_3(v)] \\
&= \sum_{v \in V} d_v^3 + d_v N_2(v) + d_v N_3(v) \\
&\qquad + d_v^2 N_2(v) + N_2(v)^2 + N_2(v) N_3(v) \\
&= \left[\sum_{v \in V} d_v^3\right] + p_2 + p_3 + p_3 + p_4 \\
&\qquad + \left[\sum_{v \in V} d_v^2 N_2(v)\right] + p_2 + p_4 \\
&\qquad + \left[\sum_{v \in V} d_v(d_v-1)(d_v-2)\right] + p_3 + p_5 \\
&\qquad + \left[\sum_{v \in V} N_2(v)(d_v-1)(d_v-2)\right] \\
&= \Bigg[\sum_{v \in V} d_v^3 + d_v^2 N_2(v) + d_v(d_v-1)(d_v-2) \\
&\qquad + N_2(v)(d_v-1)(d_v-2)\Bigg] \\
&\qquad + 2p_2 + 3p_3 + 2p_4 + p_5
\end{aligned}$$

Accordingly, this results in

$$\begin{aligned}
&w_0w_5 - w_1w_4\\
&= nw_5 - 2(n-1)w_4 = n[w_5 - 2w_4] + 2w_4\\
&= n\Bigg[\left(\sum_{v\in V}(d_v + N_2(v))\left(d_v^2 + (d_v-1)(d_v-2)\right)\right)\\
&\quad +2p_2 + 3p_3 + 2p_4 + p_5 - w_2 - 3p_2 - 2p_3 - p_4\\
&\quad -\left(\sum_{v\in V} d_v(d_v-1)(d_v-2)\right)\\
&\quad -\left(\sum_{v\in V} d_v^3\right) - p_2 - 2p_3 - p_4\Bigg] + 2w_4\\
&= n\Bigg[\left(\sum_{v\in V} d_v^2 N_2(v) + N_2(v)(d_v-1)(d_v-2)\right)\\
&\quad -w_2 - 2p_2 - p_3 + p_5\Bigg] + 2w_4\\
&= n\Bigg[\left(\sum_{v\in V} N_2(v)\left(2d_v^2 - 3d_v + 2\right)\right)\\
&\quad -w_2 - 2p_2 - p_3 + p_5\Bigg] + 2w_4\\
&= n\Bigg[\left(\sum_{v\in V} N_2(v)d_v(2d_v-3)\right) - w_2 - p_3 + p_5\Bigg]\\
&\quad +2w_4
\end{aligned}$$

Lemma A.5. *Every tree with n vertices and diameter at least 3 has at least $6n$ walks of length 4.*

Proof. For the path graph of length 3 the inequality $w_4 = 26 > 24 = 6\cdot 4 = 6n$ holds.

Let B be a tree with $\operatorname{diam}(B) \geq 3$. If we attach a leaf b via edge $\{b,x\}$ to B, this leaf is the starting point of a path of length 3. There are 14 walks of length 4 that use only edges of this path and contain the edge $\{b,x\}$. Therefore, every additional node introduces at least 14 new walks of length 4.

Since every tree with diameter at least 3 can be conctructed by iteratively attaching new leaves to P_4, the lemma follows.

By application of Lemma A.5, it is sufficient to show

$$w_5 - 2w_4 + 12 = \left(\sum_{v\in V} N_2(v)d_v(2d_v-3)\right) - w_2 - p_3 + p_5 + 12 \geq 0.$$

We show this inequality by induction for all graphs having diameter at least 4, except for the $(2,n_1,n_2)$-barbell graphs with $n_2 \geq 2$. Each such graph can be constructed from a path of length 4 by iteratively adding leaves in such a way that no intermediate step results in a $(2,n_1,n_2)$-barbell graph with $n_2 \geq 2$. To this end, we observe that a graph with diameter at least 4 contains a path of length 4 with an additional leaf attached to its center or a path of length 5 if and only if it is not a $(2,n_1,n_2)$-barbell graph. Hence, we start the construction by adding a leaf either to the center or to an end node of the path of length 4.

Fact A.1. *For the path graph of length 4, we observe $w_5 - 2w_4 + 12 \geq 0$ (since $w_5 = 72$ and $w_4 = 42$).*

Now we show that the term

$$\left(\sum_{v\in V} N_2(v)d_v(2d_v-3)\right) - w_2 - p_3 + p_5$$

cannot decrease by attaching a new leaf, if the graph had diameter at least 4 before and is not a $(2,n_1,n_2)$-barbell graph with $n_2 \geq 2$.

Let $G = (V,E)$ be the original tree fulfilling these requirements, let b denote the new leaf, and let x be the unique vertex adjacent to b. Further, let $G' = (V\cup\{b\}, E\cup\{\{b,x\}\})$ denote the resulting tree where we assume that G' is not a $(2,n_1,n_2)$-barbell graph. Further, let d_v and d'_v denote the degree of node v in G or G', resp. Similarly, $N_i(v)$ and $N'_i(v)$ shall be defined.

We observe the equalities

$$\begin{aligned} w'_2 &= w_2 + 2d_x + 2 \qquad \text{and}\\ p'_i &= p_i + 2N_{i-1}(x). \end{aligned}$$

Therefore, it is sufficient to show:

$$\left[\sum_{v\in V'} N'_2(v)d'_v(2d'_v-3)\right] - \left[\sum_{v\in V} N_2(v)d_v(2d_v-3)\right] - 2d_x - 2N_2(x) + p'_5 - p_5 - 2 \geq 0$$

All nodes having distance > 2 to b contribute the same value to both sums. Hence, we obtain:

$$\begin{aligned}
&\left[\sum_{v\in V'} N'_2(v)d'_v(2d'_v-3)\right] - \left[\sum_{v\in V} N_2(v)d_v(2d_v-3)\right]\\
&= 2{d'_b}^2 N'_2(b) - 3d'_b N'_2(b)\\
&\quad + 2{d'_x}^2 N'_2(x) - 3d'_x N'_2(x) - 2d_x^2 N_2(x) + 3d_x N_2(x)\\
&\quad + \Bigg[\sum_{v\in N'_2(b)} 2{d'_v}^2 N'_2(v) - 3d'_v N'_2(v)\\
&\quad - 2d_v^2 N_2(v) + 3d_v N_2(v)\Bigg]
\end{aligned}$$

$$
\begin{aligned}
&= 2d_x - 3d_x + \big[2(d_x+1)^2 N_2(x) - 3(d_x+1)N_2(x) \\
&\quad - 2d_x^2 N_2(x) + 3d_x N_2(x)\big] \\
&\quad + \left[\sum_{v\in N_1(x)} 2d_v^2(N_2(v)+1) - 3d_v(N_2(v)+1)\right. \\
&\quad \left. - 2d_v^2 N_2(v) + 3d_v N_2(v)\right] \\
&= -d_x + 4d_x N_2(x) - N_2(x) + \left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v\right]
\end{aligned}
$$

Thus, it is sufficient to show:

$$
\begin{aligned}
& -d_x + 4d_x N_2(x) - N_2(x) + \left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v\right] \\
& -2d_x - 2N_2(x) + p_5' - p_5 - 2 \\
= \;& 4d_x N_2(x) + \left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v + 1\right] \\
& -4d_x - 3N_2(x) + p_5' - p_5 - 2 \\
= \;& (4d_x - 3)(N_2(x) - 1) + \left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v + 1\right] \\
& + p_5' - p_5 - 5 \\
\geq \;& 0
\end{aligned}
$$

Since $\mathrm{diam}(G) \geq 4$, G contains a path with 4 edges as a subgraph. Let c denote the center vertex of this path.

Case 1: $N_4(x) \neq \emptyset$. Then we have $p_5' - p_5 = 2N_4(x) \geq 2$. Since $(4d_x - 3)(N_2(x) - 1) \geq 0$, it is now sufficient to show that $\left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v + 1\right] \geq 3$. Since G has a diameter of at least 4, there must be a neighbor y of x with $d_y \geq 2$. This vertex yields at least $2\cdot 2^2 - 3\cdot 2 + 1 = 3$ (all other terms are nonnegative).

Case 2: $N_4(x) = \emptyset$. Then we have $p_5' = p_5$, $\mathrm{diam}(G) = \mathrm{diam}(G') \leq 6$, and the distance between b and c is at most 2, i.e. $x = c$ or $x \in N_1(c)$. Hence, $d_x \geq 2$ or $N_2(x) \geq 2$. Now we show:

$$
(4d_x - 3)(N_2(x) - 1) + \left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v + 1\right] - 5 \geq 0
$$

Case 2.1: $d_x \geq 2$ and $N_2(x) \geq 2$. We get:

$$
\begin{aligned}
(4d_x - 3)(N_2(x) - 1) - 5 &\geq \\
(4\cdot 2 - 3)(2 - 1) - 5 &\geq 0
\end{aligned}
$$

Case 2.2: $d_x = 1$ and $N_2(x) \geq 2$. Then the only neighbor of x must have degree $N_2(x) + 1$. We get:

$$
\begin{aligned}
& (4d_x - 3)(N_2(x) - 1) + \left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v + 1\right] - 5 \\
= \;& N_2(x) - 1 + \left[\sum_{v\in N_1(x)} 2d_v^2 - 3d_v + 1\right] - 5 \\
= \;& N_2(x) + \big[2(N_2(x)+1)^2 - 3(N_2(x)+1) + 1\big] - 6 \\
= \;& 2N_2(x)^2 + 2N_2(x) - 6 > 0.
\end{aligned}
$$

Case 2.3: $d_x \geq 2$ and $N_2(x) = 1$. Then, since $N_4(x) = \emptyset$, the diameter of G is 4, and therefore G' is a $(2, n_1, n_2)$-barbell graph for properly chosen $n_1, n_2 \in \mathbb{N} \setminus \{0\}$. This contradicts the assumption that G' is not such a graph. Thus, this case cannot occur.

Since for every tree having diameter at most three and for all $(2, n_1, n_2)$-barbell graphs the inequality $w_0 w_5 \geq w_1 w_4$ is valid as well, it holds for all trees.