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Inequalities for the Number of Walks in Trees and General Graphs and a Generalization of a Theorem of Erdős and Simonovits

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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. We provide an insight into the relations between certain combinatorial properties of graphs and (spectral) algebraical characterizations in terms of eigenvalues and eigenvectors of the adjacency matrix.

We show that the inequality $w_{2a} \cdot w_{2(a+b+c)} \geq w_{2a+c} \cdot w_{2(a+b)+c}$ is valid for all graphs, which is a generalization of the inequality $w_{2a} \cdot w_{2b} \geq w_{a+b}^2$ published by Dress and Gutman. We also show a similar sandwich theorem for the number of closed walks starting at a given vertex. Further, we prove that $w_{2\ell+pk} \cdot w_{2\ell}^{k-1} \geq w_{2\ell+p}^k$ for all $k, \ell, p \in \mathbb{N}$, which is another generalization of the inequality by Dress and Gutman and at the same time also a generalization of an inequality published by Erdős and Simonovits. Both results can be translated directly into the corresponding forms using the higher order densities instead of the number of walks.

Furthermore, we provide two families of lower bounds for the spectral radius of the adjacency matrix (in terms of the number of closed walks starting at a specified vertex) that generalize a bound published by Nosal. We also show monotonicity, i.e., the method yields better bounds with increasing walk lengths.

In the last part of the paper, we investigate several special cases w. r. t. the graph class as well as regarding the inequality. We show, that there are connected bipartite graphs as well as unconnected cycle-free graphs that violate the inequality $w_3 \geq \bar{d} \cdot w_2$. In contrast, we show that surprisingly this inequality is always satisfied for trees and we show how to construct worst-case instances (w. r. t. the difference of both sides of the inequality) for a given degree sequence. We also provide a proof for the inequality $w_5 \geq \bar{d} \cdot w_4$ for trees and conclude with a corresponding conjecture for longer walks.

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 this number equals the number of walks of length k that start at vertex y and end at vertex 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.

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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 for arbitrary graphs $G = (V, E)$ and all vertices $x, z \in V$ holds

$$w_{k+\ell}(x, z) = \sum_{y \in V} w_k(x, y) \cdot w_\ell(y, z)$$

This implies a whole bunch of different equalities according to walk decompositions into two or more segments, for instance $w_{k+1}(x) = \sum_{y \in N(x)} w_k(y)$, $w_{k+1} = \sum_{x \in V} d_x w_k(x)$, $w_{k+\ell} = \sum_{x \in V} w_k(x) \cdot w_\ell(x)$, $w_{2k+1} = 2 \sum_{\{x,y\} \in E} w_k(x) \cdot w_k(y)$, $w_{k+\ell+1} = \sum_{\{x,y\} \in E} w_k(x) \cdot w_\ell(y) + w_k(y) \cdot w_\ell(x)$ and so on.

1.2 The spectral approach to the number of walks

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 $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$. The other way round, 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 $U^{-1} = U^T$). For convenience, let $\hat{u}_{xyi}$ denote the product $u_{xi} u_{yi}$. We also define the following abbreviation for the column sums of U:

$$B_i = \sum_{x=1}^{n} u_{xi}$$

Since U is an orthonormal matrix, we know that its column and row vectors have unit length

$$\forall x : \sum_{i=1}^{n} u_{xi}^2 = \sum_{i=1}^{n} \hat{u}_{xxi} = 1 \qquad \text{as well as} \qquad \forall y : \sum_{i=1}^{n} u_{iy}^2 = 1$$

and they are pairwise orthogonal:

$$x \neq y : \qquad \sum_{i=1}^{n} u_{xi} u_{yi} = \sum_{i=1}^{n} \hat{u}_{xyi} = 0 \qquad \text{as well as} \qquad \sum_{i=1}^{n} u_{ix} u_{iy} = 0$$

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.

The number of walks between given vertices is therefore

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

while the number of walks starting at a given vertex is

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

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 $U^T AU = D = \text{diag}(\lambda_1 \dots \lambda_n)$ it can be seen that the i-th eigenvalue λ_i and (unit) eigenvector $(u_{1i} \dots u_{ni})^T$ satisfy $\lambda_i = \sum_{(x,y)\in E} u_{xi}u_{yi}$. An even more general statement follows from $U^T A^k U = (U^T AU)^k = D^k = \text{diag}(\lambda_1^k \dots \lambda_n^k)$: $\lambda_i^k = \sum_{x\in V, y\in V} w_k(x,y)u_{xi}u_{yi}$. 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 $U^T AU = U^{-1}AU = D$, 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.

1.3 Related Work

One of the reasons to investigate the growth of the number of walks was a paper by Feige, Kortsarz, and Peleg [FKP01] that mentioned the following observation: The number of walks of length k in a graph of average degree $\overline{d}$ can be bounded from below in the following way:

$$n \cdot \overline{d}^k \leq w_k$$

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, the authors of [AFWZ95] and [FKP01] were not aware of the fact, that this inequality had already been conjectured by Erdős and Simonovits (and in fact Godsil, see [ES82]) more than 10 years before. At that time, Godsil noticed that the inequality can be proven using the results of Mulholland and Smith [MS59, MS60], Blakley and Roy [BR65], and London [Lon66]. Since $\overline{d} = 2m/n = w_1/w_0$, we can write this inequality in the following form:

Theorem 1 (Erdős et al.)**.** *In arbitrary undirected graphs holds for all* $k \in \mathbb{N}$*:*

$$w_1^k \leq w_0^{k-1} w_k$$

Lagarias, Mazo, Shepp, and McKay [LMSM83] posed the question for which numbers r and s the following inequality holds for all graphs:

$$w_r \cdot w_s \overset{?}{\leq} n \cdot w_{r+s}$$

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 2 (Lagarias et al.)**.** *In arbitrary 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]. Nevertheless 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. This could be very useful in situations where only asymptotic results are necessary.

Dress and Gutman [DG03] reported the following inequality:

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

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

For the proof, they applied the Cauchy-Schwarz inequality to the number of walks (using the combinatorial approach): $\left(\sum_{x\in V} w_a(x) \cdot w_b(x)\right)^2 \leq \left(\sum_{x\in V} w_a(x)^2\right)\left(\sum_{x\in V} w_b(x)^2\right)$, i.e., $w_{a+b}^2 \leq w_{2a} \cdot w_{2b}$. Alternatively, the inequality can be proven using the spectral approach (also using the Cauchy-Schwarz inequality): $\left[\sum_{i=1}^n \left(B_i\lambda_i^a \cdot B_i\lambda_i^b\right)\right]^2 \leq \left(\sum_{i=1}^n \left(B_i\lambda_i^a\right)^2\right)\left(\sum_{i=1}^n \left(B_i\lambda_i^b\right)^2\right)$, which implies by the intermediate step

$\left(\sum_{i=1}^{n} B_i^2 \lambda_i^{a+b}\right)^2 \leq \left(\sum_{i=1}^{n} B_i^2 \lambda_i^{2a}\right)\left(\sum_{i=1}^{n} B_i^2 \lambda_i^{2b}\right)$ that $w_{a+b}^2 \leq w_{2a} \cdot w_{2b}$. Note that all involved numbers are real numbers.

Regarding the sums of powers of the degrees, de Caen [dC98] proved that for $n \geq 2$ holds

$$w_2 = \sum_{x \in V} d_v^2 \leq m\left(\frac{2m}{n-1} + n - 2\right).$$

Nikiforov [Nik07] showed that

$$\sum_{i=1}^{n} d_i^2 \leq \begin{cases} (2m)^{3/2} & \text{for } m \geq n^2/4 \\ (n^2 - 2m)^{3/2} + 4mn - n^3 & \text{for } m < n^2/4 \end{cases}$$

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

The lower bound for the largest eigenvalue of the adjacency matrix $\lambda_1 \geq \overline{d} = 2m/n = w_1/w_0$ by Collatz and Sinogowitz [CS57] was generalized by Nikiforov [Nik06] to

$$\frac{w_{k+r}}{w_k} \leq \lambda_1^r$$

for all $r \geq 1$ and *even* numbers $k \geq 0$. 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. 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:

$$\frac{w_r}{n} \leq \lambda_1^r \qquad \text{and} \qquad \frac{w_{2\ell+1}}{w_{2\ell}} \leq \lambda_1$$

which also contains the bound of Collatz and Sinogowitz as a special case.

Furthermore, 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: $\sqrt{\Delta} \leq \lambda_1$ (also mentioned without proof in Lovász and Pelikan [LP73] as well as in [CR90]). For a survey of bounds of the largest eigenvalue, see [CR90].

2 Generalized inequalities for the number of walks of length k and for the k-th order density

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

Theorem 2 (the inequality of Lagarias et al.) and Theorem 3 (the inequality of Dress and Gutman) are special cases of the following inequality:

Theorem 4 (Sandwich Theorem)**.** *Let $G = (V, E)$ be an undirected graph.*
Then for all $a, b, c \in \mathbb{N}$ and $v \in V$ holds:

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

and

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

Proof. Assume that $\lambda_1 \geq \ldots \geq \lambda_n$ and that p_i is a nonnegative value for all i. Then all of the following lines are equivalent:

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

Each of the summands 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. Setting $p_i = B_i^2$ yields $0 \leq w_{2a} \cdot w_{2(a+b+c)} - w_{2a+c} \cdot w_{2a+2b+c}$ and setting $p_i = u_{v,i}^2$ yields $0 \leq w_{2a}(v,v) \cdot w_{2(a+b+c)}(v,v) - w_{2a+c}(v,v) \cdot w_{2a+2b+c}(v,v)$. $\square$

2.2 The density implication

For a graph G having n vertices and m edges a density ρ can be 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 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 4 directly implies the following inequality:

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

Corollary 5. *For all $a, b, c \in \mathbb{N}$ holds:*

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

2.3 A unifying generalization of the inequalities of Erdős et al. and Dress & Gutman

We now show a generalization of Theorem 1 (the inequality of Erdős et al.) which is at the same time another generalization of Theorem 3 (the inequality of Dress and Gutman). The proof uses the following theorem of Blakley and Roy [BR65] (which is essentially the same idea as in the comment of the Erdős / Simonovits paper).

Lemma 6. *Let $U_n = \{u \in \mathbb{R}_n : \langle u, u \rangle = 1\}$ denote the n-dimensional unit sphere.*

If S is a nonnegative symmetric $n \times n$ matrix, $u \in U_n$ is nonnegative and k is a positive integer then $\langle u, Su \rangle^k \leq \langle u, S^k u \rangle$.

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 $k+2\ell$.

The length of this vector is $||\vec{w}_\ell|| = \sqrt{\sum_{v\in V}^n w_\ell(v)^2} = \sqrt{w_{2\ell}}$. Now, assuming that $||\vec{w}_\ell|| \neq 0$, application of Lemma 6 to the matrix $S = A^p$ and the unit vector $u = \vec{w}_\ell/||\vec{w}_\ell||$ yields

$$\begin{aligned}
\left\langle \frac{1}{||\vec{w}_\ell||}\vec{w}_\ell, A^p \frac{1}{||\vec{w}_\ell||}\vec{w}_\ell \right\rangle^k &\leq \left\langle \frac{1}{||\vec{w}_\ell||}\vec{w}_\ell, A^{pk} \frac{1}{||\vec{w}_\ell||}\vec{w}_\ell \right\rangle \\
\left\langle \frac{1}{\sqrt{w_{2\ell}}}\vec{w}_\ell, A^p \frac{1}{\sqrt{w_{2\ell}}}\vec{w}_\ell \right\rangle^k &\leq \left\langle \frac{1}{\sqrt{w_{2\ell}}}\vec{w}_\ell, A^{pk} \frac{1}{\sqrt{w_{2\ell}}}\vec{w}_\ell \right\rangle \\
\left(\frac{w_{2\ell+p}}{w_{2\ell}}\right)^k &\leq \frac{w_{2\ell+pk}}{w_{2\ell}}
\end{aligned}$$

Theorem 7. *The following inequality is valid for arbitrary graphs and $k, \ell, p \in \mathbb{N}$:*

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

For all graphs with at least one edge this is equivalent to

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

Setting $k=2$ leads to $w_{2\ell+p}^2 \leq w_{2\ell+2p} \cdot w_{2\ell}$ and therefore results in inequality 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 8. *For arbitrary graphs and $k, p \in \mathbb{N}$ holds*

$$w_p^k \leq n^{k-1} w_{pk} \qquad \textit{or} \qquad \left(\frac{w_p}{n}\right)^k \leq \frac{w_{pk}}{n}$$

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 inequality 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, assuming that $||\vec{w}_\ell(v)|| \neq 0$, the application of Lemma 6 yields

$$\begin{aligned}
\left\langle \frac{1}{||\vec{w}_\ell(v)||}\vec{w}_\ell(v), A^p \frac{1}{||\vec{w}_\ell(v)||}\vec{w}_\ell(v) \right\rangle^k &\leq \left\langle \frac{1}{||\vec{w}_\ell(v)||}\vec{w}_\ell(v), A^{pk} \frac{1}{||\vec{w}_\ell(v)||}\vec{w}_\ell(v) \right\rangle \\
\left\langle \frac{1}{\sqrt{w_{2\ell}(v,v)}}\vec{w}_\ell(v), A^p \frac{1}{\sqrt{w_{2\ell}(v,v)}}\vec{w}_\ell(v) \right\rangle^k &\leq \left\langle \frac{1}{\sqrt{w_{2\ell}(v,v)}}\vec{w}_\ell(v), A^{pk} \frac{1}{\sqrt{w_{2\ell}(v,v)}}\vec{w}_\ell(v) \right\rangle \\
\left(\frac{w_{2\ell+p}(v,v)}{w_{2\ell}(v,v)}\right)^k &\leq \frac{w_{2\ell+pk}(v,v)}{w_{2\ell}(v,v)}
\end{aligned}$$

Theorem 9. *The following inequality regarding the number of closed walks is valid for each vertex v in arbitrary graphs and for all $k, \ell, p \in \mathbb{N}$:*

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

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

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

2.4 The density implication

Theorem 7 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 10. *For arbitrary graphs and* $k, \ell, p \in \mathbb{N}$ *holds:* $\rho_{2\ell+p}^k \leq \rho_{2\ell+pk} \cdot \rho_{2\ell}$
This includes the following special cases: $\rho_p^k \leq \rho_{pk} \quad (\ell = 0)$ *and* $\rho^k \leq \rho_k \quad (\ell = 0, p = 1)$

3 Generalization of a lower bound for the spectral radius

We now show a generalization of the following lower bound for the largest eigenvalue that was shown by Nosal [Nos70]: $\sqrt{\Delta} \leq \lambda_1$.

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 well-known Rayleigh-Ritz Theorem leads to an even more general lower bound for the spectral radius of graphs.

Theorem 11 (Rayleigh-Ritz Theorem)**.** *Let* $A \in \mathbb{C}^{n \times n}$ *be a Hermitian matrix. Then its 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 12. *For arbitrary graphs, the spectral radius* λ_1 *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.

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:

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

Lemma 13. *For $k, \ell, x, y \in \mathbb{N}$ with $k \geq 1$ holds*

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

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., $\sqrt[k+1]{\frac{w_{2(k+1)+2\ell}(v,v)}{w_{2\ell}(v,v)}} = F^2_{k+1,\ell} \geq F^2_{k,\ell} = \sqrt[k]{\frac{w_{2k+2\ell}(v,v)}{w_{2\ell}(v,v)}}$.

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

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

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., $\sqrt[k]{\frac{w_{2k+2(\ell+1)}(v,v)}{w_{2(\ell+1)}(v,v)}} = F^2_{k,\ell+1} \geq F^2_{k,\ell} = \sqrt[k]{\frac{w_{2k+2\ell}(v,v)}{w_{2\ell}(v,v)}}$. 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 9 and 7 directly imply additional monotonicity results for our new bound, as well as for Nikiforov's bound:

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

In contrast to Lemma 13, these inequalities provide a monotonicity statement for certain *odd* walk lengths, too.

4 Counterexamples for special cases

4.1 Bipartite graphs

Since we assume the validity of the rigorous inequality for all trees, it would be interesting to prove or disprove validity for more general graph classes that contain the class of all trees or forests, e.g. the class of all bipartite graphs.

We will show, that there are arbitrarily large bipartite graphs that violate the rigorous inequality. Similar to the general counterexamples proposed in [LMSM84], our counterexamples consist of two parts: a star and (instead of complete graphs) complete bipartite graphs. The respective number of walks are:

$$\begin{array}{rclrl} w_0(B_{n/2,n/2}) &=& n & w_0(S_n)= & n \\ w_1(B_{n/2,n/2}) &=& n\cdot\left(\frac{n}{2}\right) & w_1(S_n)= & 2(n-1) \\ w_2(B_{n/2,n/2}) &=& n\cdot\left(\frac{n}{2}\right)^2 & w_2(S_n)= & n(n-1) \\ w_3(B_{n/2,n/2}) &=& n\cdot\left(\frac{n}{2}\right)^3 & w_3(S_n)= & 2(n-1)^2 \end{array}$$

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: $w_0 w_3 = 820 \not\geq 828 = w_1 w_2$. This way we found an even smaller (disconnected) counterexample. Connected counterexamples can be constructed by 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 $n \geq 3$):

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

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

$$\begin{array}{rcl} (x+y)(2\cdot(x-1)^2 + 8y - 16) &\geq& (x(x-1) + 4y - 6)(2(x-1) + 2(y-1)) \\ x^2 - 3x - xy + 7y - 12 &\geq& 0 \end{array}$$

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}.

4.3 Trees

Most surprisingly, the connected variant is no longer a counterexample. We define the *comet graph* $Co_{x,y}$ to consist of a star (having x nodes) and a path (having y nodes), where the center of the star is connected to an end vertex of the path through another edge.

$$\begin{array}{ll} w_0(Co_{x,y}) = x + y & = x + y \\ w_1(Co_{x,y}) = 2\cdot(x-1+1+y-1) & = 2x + 2y - 2 \\ w_2(Co_{x,y}) = (x-1)\cdot 1^2 + x^2 + (y-1)\cdot 2^2 + 1\cdot 1^2 & = x^2 + x + 4y - 4\ (y > 1) \\ w_3(Co_{x,y}) = 2[(x-1)\cdot 1\cdot x + 1\cdot 2\cdot x + (y-2)\cdot 2\cdot 2 + 1\cdot 1\cdot 2] & = 2[(x+1)x + 4y - 6] \end{array}$$

$$\begin{array}{rcl} (x+y)\cdot 2[(x+1)x + 4y - 6] &\geq& (x^2 + x + 4y - 4)\cdot 2(x+y-1) \\ x^2 - x + 2y - 4 &\geq& 0 \quad \text{(no contradiction!)} \end{array}$$

Thus, the former counterexample consisting of a star and a path does not work in the connected case.

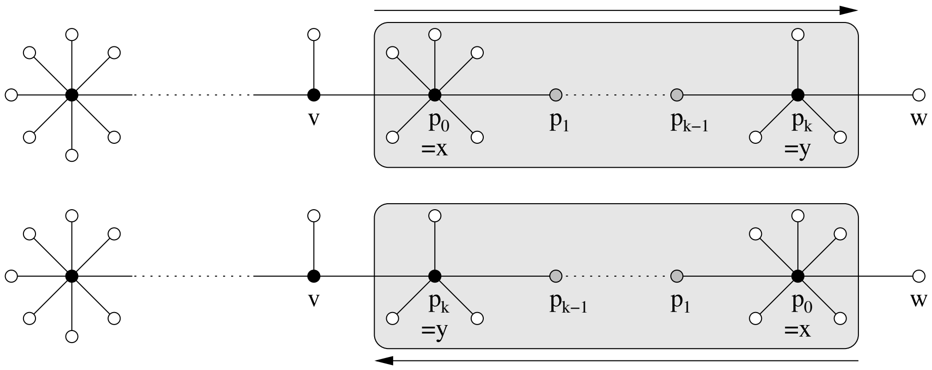

Figure 1: Path inversion in a (caterpillar) tree

4.4 Construction of worst case trees

In order to answer the question whether the inequality $w_0w_3 \geq w_1w_2$ holds for all trees we investigate the behavior of different trees with respect to the value of the difference of both sides, i.e. $w_0w_3 - w_1w_2$. 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.

Lemma 14. *For a given degree sequence of a tree, the tree that minimizes the value of the difference $w_0w_3 - w_1w_2$ cannot have four different vertices $v, w, x, y \in V$ such that*

- *x and y are the neighbors of v and w (resp.) on the path from v to w.*
- *$d_x > d_y$ and $d_v > d_w$*

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 $d_y d_v + d_x d_w$.

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

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 $w_0w_3 - w_1w_2$ was a minimum. □

At first, we have a look at a special class of trees, namely the caterpillar trees.

Definition 15. *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 $nw_3 - w_2w_1$ 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 $nw_3 - w_2 w_1$): 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 of the path.

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

Within this subsection we only consider trees.

5.1 Stars

Lemma 16. *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 have $w_{2k} = n(n-1)^k$ 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, we get $2(n-1)^{(k-1)/2+1} \cdot 2(n-1)^{(\ell-1)/2+1} = 4(n-1)^{(k+\ell)/2+1} \leq n \cdot n(n-1)^{(k+\ell)/2}$ 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 $w_{a+b} \cdot w_{a+c} \leq w_a \cdot w_{a+b+c}$. By contrast, if all parameters a, b, c are odd numbers, the relation symbol of the inequality is inverted.

5.2 Paths

Lemma 17. *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 we have

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

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. □

5.3 The w_3-inequality for trees

Let $N_i(v)$ denote the set of all nodes w having distance $d(v, w) = i$. Further, let p_i denote the number of (directed) paths (i.e., vertex-disjoint walks) of length i.

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

$$\begin{aligned}
w_1 &= 2(n-1) \\
w_2 &= \sum_{v \in V} d_v + N_2(v) = w_1 + 2p_2 = 2(n-1) + p_2 \\
w_3 &= \sum_{v \in V} d_v^2 + N_2(v) + N_3(v) = w_2 + p_2 + p_3 = 2(n-1) + 2p_2 + p_3
\end{aligned}$$

Theorem 18. *For all trees the following inequality is valid:* $\quad w_1 \cdot w_2 \leq w_0 \cdot w_3$.

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

$$\begin{aligned}
w_0 w_3 - w_1 w_2 &= nw_3 - 2(n-1)w_2 = n(w_3 - 2w_2) + 2w_2 \\
&= n[p_3 - 2n + 6] + 2(p_2 - 2)
\end{aligned}$$

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 16).

Let $G = (V, E)$ be any tree that satisfies the conditions $\mathrm{diam}(G) \geq 3$, $(p_3 - 2n + 6) \geq 0$ 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. □

5.4 Trees with diameter 3 (barbell graphs)

Definition 19. *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 $n_2 \geq n_1$ leafs at the two end vertices x_1 and x_2, respectively.*

Observation 20. *Each $(1, n_1, n_2)$-barbell graph is a tree having diameter 3. Every tree with diameter 3 is a $(1, n_1, n_2)$-barbell graph for porperly chosen n_1, n_2.*

In the following, we show that for each $i \in 2\mathbb{N} \setminus \{0\}$ and for every $(1, n_1, n_2)$-barbell graph $G = (V, E)$ (and thus for all trees having diameter 3) holds:

$$\left[\sum_{v \in V} (d(v) - 2) w_i(v)\right] + 2w_i/n \geq 0$$

Let $w_{i,j}(v)$ be the number of walks starting at $v \in V$ and having length i, where the last part is a *path* of length j.

Observation 21. *For each vertex $v \in V$ and all $i \in \mathbb{N} \setminus \{0\}$ holds $w_{i+1}(v) = w_i(v) + w_{i+1,2}(v)$*

Lemma 22. *For each $(1, n_1, n_2)$-barbell graph and every $i \in 2\mathbb{N} + 1$ 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.

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 $i' < i$, then we have:

$$\begin{aligned} w_i(x_1) &= w_{i-1}(x_2) + n_1 w_{i-1}(b_1) = w_{i-1}(x_2) + n_1 w_{i-2}(x_1) \\ &\leq w_{i-1}(x_2) + n_2 w_{i-2}(x_2) = w_{i-1}(x_2) + w_{i,2}(x_2) = w_i(x_2) \end{aligned}$$

The inequality follows from $n_1 \leq n_2$, Observation 21 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 23. *For each $(1, n_1, n_2)$-barbell graph and every $i \in 2\mathbb{N} \setminus \{0\}$ 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 $2w_i/n \geq w_{i-1}(x_1) + w_{i-1}(x_2)$. To this end we find by Observation 21 that the number of i-walks starting at a leaf of x_1 (or x_2, resp.) or vertex x_1 (or x_2, resp.) itself is not smaller than the number of $(i-1)$-walks starting at x_1 (or x_2, resp.). Since $n_1 \leq n_2$ and by applying Lemma 22 we get:

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

□

5.5 $(2, n_1, n_2)$-barbell graphs

Lemma 24. *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 25. *For each $(2, n_1, n_2)$-barbell graph and every $i \in 2\mathbb{N} \setminus \{0\}$ 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 $2w_i/n \geq w_{i-1}(x_1) + w_{i-1}(x_2)$. We conclude that due to Observation 21 the number of i-walks starting at a leaf of x_1 (or x_2, resp.) or at x_1 (or x_2, resp.) itself is at least the number of $(i-1)$-walks starting at x_1 (or x_2, resp.) 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 24 (applied to x_1 and x_2) we get:

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

Remark without proof: In the inequalities above, each "$\geq$"-symbol can be replaced by "$>$". ☐

5.6 The w_5-inequality for trees

Theorem 26. *For all trees the following inequality is valid:* $w_1 \cdot w_4 \leq w_0 \cdot w_5$.

Proof. In the following, let $G = (V, E)$ be a tree. For each $i \in \mathbb{N}_0$ holds the following equivalence:

$$\begin{aligned}
nw_{i+1} - 2(n-1)w_i &= \left[n \cdot \sum_{v\in V}(d(v)-2)w_i(v)\right] + 2w_i \geq 0 \\
\Leftrightarrow \left[\sum_{v\in V}(d(v)-2)w_i(v)\right] &+ 2w_i/n \geq 0
\end{aligned}$$

Therefore, every i-walk that starts at a leaf creates a negative unit that has to be compensated for by the contribution of the other vertices and the correction term $2w_i/n$ if we want to prove the inequality.

From Observation 21 follows:

Lemma 27. *Let b be a leaf attached at an inner vertex x. Then we have*

$$(\deg(x)-2)w_{i+2}(x) = (\deg(x)-2)(w_{i+1}(x) + w_{i+2,2}(x) \geq (\deg(x))-2)w_{i+2}(b)$$

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 leafs. This is called deficit adjustment at node x.

Besides $w_0(v) = 1$, $w_1(v) = d(v)$, $w_2(v) = d(v) + N_2(v)$, and $w_3(v) = d(v)^2 + N_2(v) + N_3(v)$ we know

$$
\begin{aligned}
\sum_{v\in V} d(v)^2 &= w_2 \\
\sum_{v\in V} d(v)N_2(v) &= p_2 + p_3 \\
\sum_{v\in V} d(v)N_3(v) &= p_3 + p_4 \\
\sum_{v\in V} N_2(v)^2 &= p_2 + p_4 + \sum_{v\in V} d(v)(d(v)-1)(d(v)-2) \\
\sum_{v\in V} N_2(v)N_3(v) &= p_3 + p_5 + \sum_{v\in V} N_2(v)(d(v)-1)(d(v)-2)
\end{aligned}
$$

$$
\begin{aligned}
w_2 =& \sum_{v\in V} w_2(v) = \sum_{v\in V}[d(v) + N_2(v)] \\
w_3 =& \sum_{v\in V} w_3(v) = \sum_{v\in V}[d(v)^2 + N_2(v) + N_3(v)] \\
w_4 =& \sum_{v\in V} w_2(v)^2 = \sum_{v\in V}[d(v) + N_2(v)]^2 = \sum_{v\in V}[d(v)^2 + 2d(v)N_2(v) + N_2(v)^2] \\
&= w_2 + 2p_2 + 2p_3 + p_2 + p_4 + \sum_{v\in V} d(v)(d(v)-1)(d(v)-2) \\
&= w_2 + 3p_2 + 2p_3 + p_4 + \sum_{v\in V} d(v)(d(v)-1)(d(v)-2) \\
=& \sum_{v\in V} w_1(v)w_3(v) = \sum_{v\in V} d(v)\cdot[d(v)^2 + N_2(v) + N_3(v)] \\
&= \sum_{v\in V}[d(v)^3 + d(v)N_2(v) + d(v)N_3(v)] \\
&= \sum_{v\in V}[d(v)^3] + p_2 + 2p_3 + p_4 \\
w_5 =& \sum_{v\in V} w_2(v)w_3(v) = \sum_{v\in V}[d(v) + N_2(v)]\cdot[d(v)^2 + N_2(v) + N_3(v)] \\
&= \sum_{v\in V}[d(v)^3 + d(v)N_2(v) + d(v)N_3(v) + d(v)^2N_2(v) + N_2(v)^2 + N_2(v)N_3(v)] \\
&= \sum_{v\in V}[d(v)^3] + p_2 + p_3 + p_3 + p_4 + \sum_{v\in V}[d(v)^2N_2(v)] + p_2 + p_4 \\
&+ \sum_{v\in V}[d(v)(d(v)-1)(d(v)-2)] + p_3 + p_5 + \sum_{v\in V}[N_2(v)(d(v)-1)(d(v)-2)] \\
&= \sum_{v\in V}[d(v)^3 + d(v)^2N_2(v) + d(v)(d(v)-1)(d(v)-2) + N_2(v)(d(v)-1)(d(v)-2)] \\
&+ 2p_2 + 3p_3 + 2p_4 + p_5
\end{aligned}
$$

Therefore,

$$\begin{aligned}
w_0w_5 - w_1w_4 = n \cdot &\Bigg[\sum_{v\in V}[d(v)^3 + d(v)^2N_2(v) + d(v)(d(v)-1)(d(v)-2) + N_2(v)(d(v)-1)(d(v)-2)] \\
&+ 2p_2 + 3p_3 + 2p_4 + p_5] \\
&- n \cdot \Bigg[w_2 + 3p_2 + 2p_3 + p_4 + \sum_{v\in V}[d(v)(d(v)-1)(d(v)-2)] \\
&+ \sum_{v\in V}[d(v)^3] + p_2 + 2p_3 + p_4\Bigg] + 2w_4 \\
= n \cdot &\left[\sum_{v\in V}[d(v)^2N_2(v) + N_2(v)(d(v)-1)(d(v)-2)] + 2p_2 + 3p_3 + 2p_4 + p_5\right] \\
&- n \cdot [w_2 + 4p_2 + 4p_3 + 2p_4] + 2w_4 \\
= n \cdot &\left[\sum_{v\in V}[d(v)^2N_2(v) + N_2(v)(d(v)-1)(d(v)-2)] - w_2 - 2p_2 - p_3 + p_5\right] + 2w_4
\end{aligned}$$

Lemma 28. *Every tree with n vertices and diameter at least 3 has at least $6n$ walks of length 4.*

Proof. For the path graph P_4 holds $w_4(P_4) = 26 > 24 = 6 \cdot 4 = 6 \cdot n(P_4)$.

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 28, it is sufficient to show the following inequality:

$$[w_5 - 2w_4 + 12 =] \quad \sum_{v\in V}[d(v)^2N_2(v) + N_2(v)(d(v)-1)(d(v)-2)] - w_2 - 2p_2 - p_3 + p_5 + 12 \geq 0$$

Observation 29. *For a path graph having 4 edges, we have $w_5 - 2w_4 + 12 \geq 0$ (since $w_5 = 72$ and $w_4 = 42$).*

Now we show that the term

$$\sum_{v\in V}[d(v)^2N_2(v) + N_2(v)(d(v)-1)(d(v)-2)] - w_2 - 2p_2 - p_3 + p_5$$

cannot decrease by attaching a new leaf, if the graph had diameter at least 4 before.

Let $G = (V, E)$ be the original tree with $\operatorname{diam}(G) \geq 4$, 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 and let $d(v)$ and $d'(v)$ denote the degree of node v in G or G', resp. Similarly, $N_i(v)$ and $N'_i(v)$ should be defined.

We know:

$$\begin{aligned}
w'_2 &= w_2 + 2d(x) + 2 \\
p'_2 &= p_2 + 2d(x) \\
p'_3 &= p_3 + 2N_2(x)
\end{aligned}$$

Therefore, it is sufficient to show:

$$\sum_{v\in V'}[d'(v)^2N_2'(v)+N_2'(v)(d'(v)-1)(d'(v)-2)]-\sum_{v\in V}[d(v)^2N_2(v)+N_2(v)(d(v)-1)(d(v)-2)]$$
$$-6d(x)-2N_2(x)+p_5'-p_5-2\geq 0$$

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

$$\begin{aligned}
&\sum_{v\in V'}[d'(v)^2N_2'(v)+N_2'(v)(d'(v)-1)(d'(v)-2)]-\sum_{v\in V}[d(v)^2N_2(v)+N_2(v)(d(v)-1)(d(v)-2)]\\
=&\sum_{v\in V'}[2d'(v)^2N_2'(v)-3N_2'(v)d'(v)+2N_2'(v)]-\sum_{v\in V}[2d(v)^2N_2(v)-3N_2(v)d(v)+2N_2(v)]\\
=&\,2d'(b)^2N_2'(b)-N_2'(b)\\
&+\sum_{v\in N_1'(b)}[2d'(v)^2N_2'(v)-3N_2'(v)d'(v)+2N_2'(v)-2d(v)^2N_2(v)+3N_2(v)d(v)-2N_2(v)]\\
&+\sum_{v\in N_2'(b)}[2d'(v)^2N_2'(v)-3N_2'(v)d'(v)+2N_2'(v)-2d(v)^2N_2(v)+3N_2(v)d(v)-2N_2(v)]\\
=&\,d(x)+[2(d(x)+1)^2N_2(x)-3N_2(x)(d(x)+1)+2N_2(x)-2d(x)^2N_2(x)+3N_2(x)d(x)-2N_2(x)]\\
&+\sum_{v\in N_1(x)}[2d(v)^2(N_2(v)+1)-3(N_2(v)+1)d(v)+2(N_2(v)+1)-2d(v)^2N_2(v)+3N_2(v)d(v)-2N_2(v)]\\
=&\,d(x)+[4d(x)N_2(x)+2N_2(x)-3N_2(x)]+\sum_{v\in N_1(x)}[2d(v)^2-3d(v)+2]\\
=&\,d(x)+4d(x)N_2(x)-N_2(x)+\sum_{v\in N_1(x)}[2d(v)^2-3d(v)+2]
\end{aligned}$$

Thus, it is sufficient to show:

$$\begin{aligned}
&d(x)+4d(x)N_2(x)-N_2(x)+\sum_{v\in N_1(x)}[2d(v)^2-3d(v)+2]-6d(x)-2N_2(x)+p_5'-p_5-2\\
&=4d(x)N_2(x)+\sum_{v\in N_1(x)}[2d(v)^2-3d(v)+2]-5d(x)-3N_2(x)+p_5'-p_5-2\\
&=4d(x)N_2(x)+\sum_{v\in N_1(x)}[2d(v)^2-3d(v)+1]-4d(x)-3N_2(x)+p_5'-p_5-2\geq 0
\end{aligned}$$

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 0: G is a $(2,n_1,n_2)$-barbell graph, but G is not a path graph and $x=c$. Then, we attach b to x (getting G') and cut out a leaf $b'\neq b$ with $N_2(b')\geq 2$ from G', resulting in graph G''. Note that G'' is not a $(2,n_1',n_2')$-barbell graph, but it still has diameter 4. Now we treat b'' as b and G'' as G and proceed with one of the following cases.

Case 1: $N_4(x) \neq \emptyset$. Then we have $p'_5 - p_5 - 2 \geq 0$. Since G has a diameter of at least 4, there must be a neighbor y of x with $d_y \geq 2$. Thus we get:

$$\begin{aligned}
&4d(x)N_2(x) + \sum_{v \in N_1(x)} [2d(v)^2 - 3d(v) + 1] - 4d(x) - 3N_2(x) \\
&\geq 4d(x)N_2(x) + \sum_{v \in N_1(x) - \{y\}} [2d(v)^2 - 3d(v) + 1] + 3 - 4d(x) - 3N_2(x) \\
&\geq 4d(x)N_2(x) + 3 - 4d(x) - 3N_2(x)
\end{aligned}$$

For $d(x) = 1$ or $N_2(x) = 1$, the term is nonnegativ. For $d(x) \geq 2$ and $N_2(x) \geq 2$ holds:

$$\begin{aligned}
&4d(x)N_2(x) + 3 - 4d(x) - 3N_2(x) = [2d(x)N_2(x) - 4d(x)] + [2d(x)N_2(x) - 3N_2(x)] + 3 \\
&\geq [4d(x) - 4d(x)] + [4N_2(x) - 3N_2(x)] + 3 > 0
\end{aligned}$$

Case 2: $N_4(x) = \emptyset$. Then we have $\operatorname{diam}(G) = \operatorname{diam}(G') \leq 6$ and $d(b, c) \leq 2$, as well as $p'_5 = p_5$. Hence, $d(x) \geq 2$ or $N_2(x) \geq 2$. Now we show:

$$4d(x)N_2(x) + \sum_{v \in N_1(x)} [2d(v)^2 - 3d(v) + 1] - 4d(x) - 3N_2(x) - 2 \geq 0$$

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

$$\begin{aligned}
&4d(x)N_2(x) + \sum_{v \in N_1(x)} [2d(v)^2 - 3d(v) + 1] - 4d(x) - 3N_2(x) - 2 \\
&\geq 4d(x)N_2(x) - 4d(x) - 3N_2(x) - 2 \\
&\geq (2d(x)N_2(x) - 4d(x)) + (2d(x)N_2(x) - 3N_2(x)) - 2 \\
&\geq N_2(x) - 2 \geq 0
\end{aligned}$$

Case 2.2: $d(x) = 1$ and $N_2(x) \geq 2$. We get:

$$\begin{aligned}
&4d(x)N_2(x) + \sum_{v \in N_1(x)} [2d(v)^2 - 3d(v) + 1] - 4d(x) - 3N_2(x) - 2 \\
&= 4d(x)N_2(x) + [2(N_2(x) + 1)^2 - 3(N_2(x) + 1) + 1] - 4d(x) - 3N_2(x) - 2 \\
&= 4N_2(x) + [2N_2(x)^2 + 4N_2(x) + 2 - 3N_2(x) - 3 + 1] - 6 - 3N_2(x) \\
&= 2N_2(x) + 2N_2(x)^2 - 6 > 0
\end{aligned}$$

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 $n_1, n_2 \in \mathbb{N} \setminus \{0\}$, for which $w_0 w_5 \geq w_1 w_4$ holds.

Since for every tree having diameter at most three, the inequality $w_0 w_5 \geq w_1 w_4$ is valid as well, this inequality holds for all trees. $\square$

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

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

(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. As it turns out, this case of an *odd* index on the greater side is equivalent to a statement about averages:

$$\begin{aligned} w_{2k}/w_0 &\leq w_{2k+1}/w_1 \\ \frac{1}{n}\sum_{x \in V} w_k(x)^2 &\leq \frac{1}{m}\sum_{\{x,y\} \in E} w_k(x) \cdot w_k(y) \end{aligned}$$

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