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Further Results on the Number of Walks in Graphs and Weighted Entry Sums of Matrix Powers

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Abstract

We consider the number of walks in undirected and directed graphs and, more generally, the weighted sum of entries of matrix powers. In this respect, we generalize an earlier result for Hermitian matrices. By using these inequalities for the entry sum of matrix powers, we deduce similar inequalities for iterated kernels. For further conceivable inequalities, we provide counterexamples in the form of graphs that contradict the corresponding statement for the number of walks. For the largest eigenvalue of adjacency matrices, we generalize a bound of Nikiforov that uses the number of walks. Furthermore, we relate the number of walks in graphs to the number of nodes and the number of edges in iterated directed line graphs.

1 Introduction

1.1 Notation

We use standard notation, where $\mathbb{R}$ denotes the set of real numbers, $\mathbb{C}$ is the set of complex numbers, $\mathbb{N}$ denotes the set of nonnegative integers, and $[n]$ is the set $\{1, \ldots, n\}$. The n-dimensional vector where each entry is 1 is denoted by $\mathbf{1}$.

Throughout the paper, A denotes an $n \times n$-matrix with entries $a_{i,j} \in \mathbb{C}$. We refer to the entry in row i and column j of a matrix A (i.e., $A_{(i,j)} = a_{i,j}$) as the (i,j)-entry of A. The transpose of matrix A is denoted by A^T, i.e., $(A^T)_{(i,j)} = A_{(j,i)}$. For $c = a + ib \in \mathbb{C}$ with $a, b \in \mathbb{R}$, $\bar{c} = a - ib$ denotes the complex conjugate of c. The conjugate transpose of the matrix A is denoted by A^*, i.e., $(A^*)_{(i,j)} = \bar{A}_{(j,i)}$. The (i,j)-entry of the k-th matrix power A^k is denoted by $a_{i,j}^{[k]} = \left(A^k\right)_{(i,j)}$. The sum of all entries in row i and column j is denoted by r_i and c_j, respectively. For the total sum of all entries of A, we use the notation $\mathrm{sum}(A) = \sum_{i\in[n]} \sum_{j\in[n]} a_{i,j}$.

Let $G = (V, E)$ be a (directed or undirected) graph having n vertices and m edges. Unless stated otherwise, we assume that the graph is simple and there are no loops. An undirected edge between vertices u and v is denoted by the unordered pair $\{u, v\}$. In contrast, a directed edge from u to v is denoted by the ordered pair (u, v). The out-degree of node x (the number of edges emanating from x) is denoted by $d_{\mathrm{out}}(x)$ while the in-degree of x (the number of edges pointing to x) is denoted by $d_{\mathrm{in}}(x)$. For undirected graphs, we use $d_x = d_{\mathrm{out}}(x) = d_{\mathrm{in}}(x)$. The adjacency matrix A of G is the $n \times n$-matrix where $a_{i,j} = 1$ if there is an edge from node i to node j in G, and $a_{i,j} = 0$ otherwise.

We investigate (the number of) directed 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 of a walk is the number of its edges. For vertices $x, y \in V$ and $k \in \mathbb{N}$, let $W_k(x, y)$ denote the set of walks of length k that start at vertex x and end at vertex y. Let $w_k(x, y) = |W_k(x, y)|$ denote the corresponding number of walks of length k from x to y. For undirected graphs, we have $w_k(x, y) = w_k(y, x)$. Let $s_k(x) = \sum_{y\in V} w_k(x, y)$ denote the number of walks of length k that *start* at node x. Similarly, $e_k(x) = \sum_{y\in V} w_k(y, x)$ denotes the number of walks of length k that *end* at node x. In the case of *undirected* graphs, those numbers are

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equal. Then we use the term $w_k(x) = s_k(x) = e_k(x)$. In general, $w_k = \sum_{x\in V} s_k(x) = \sum_{x\in V} e_k(x)$ denotes the total number of walks of length k. Obviously, $w_k = \sum_{x\in V} w_k(x)$ holds for undirected graphs.

It is a well known fact that for every graph on n nodes with adjacency matrix A, the (i,j)-entry of A^k equals the number of walks of length k that start at vertex i and end at vertex j, i.e., $w_k(i,j) = a^{[k]}_{i,j}$ for $i,j \in [n]$ and $k \in \mathbb{N}$. This implies $s_k(i) = r^{[k]}_i$, $e_k(j) = c^{[k]}_j$ (in particular $d_{\text{out}}(i) = r_i$, $d_{\text{in}}(j) = c_j$), and in total $w_k = \text{sum}(A^k)$. For each node v, we have $s_0(v) = e_0(v) = 1$ ($w_0(v) = 1$ for undirected graphs) and $s_1(v) = d_{\text{out}}(v)$ as well as $e_1(v) = d_{\text{in}}(v)$ ($w_1(v) = d_v$ for undirected graphs). This implies $w_0 = n$ and $w_1 = m$ ($w_1 = 2m$ for undirected graphs).

A fundamental observation is that, in any directed or undirected graph, the number of walks of length $k+\ell$ from a vertex $x \in V$ to a vertex $z \in V$ can be decomposed by $w_{k+\ell}(x,z) = \sum_{y\in V} w_k(x,y)\cdot w_\ell(y,z)$. For matrices, this could be expressed as $a^{[k+\ell]}_{x,z} = \sum_{y\in[n]} a^{[k]}_{x,y}\cdot a^{[\ell]}_{y,z}$ For an arbitrary matrix A, we have $\text{sum}\left(A^{k+\ell}\right) = \sum_{i\in[n]} c^{[k]}_i \cdot r^{[\ell]}_i$. This implies for directed graphs that $w_{k+\ell} = \sum_{x\in V} e_k(x)\cdot s_\ell(x)$ and for undirected graphs that $w_{k+\ell} = \sum_{x\in V} w_k(x)\cdot w_\ell(x)$.

1.2 Motivation and Related Work

Inequalities for the entry sum of matrix powers, and in particular for the number of walks in graphs, appeared in different research subjects. Prominent examples are inapproximability results for the problems Maximum Clique and Densest k-Subgraph [AFWZ95; FKP01], extremal graph theory [ES82], spectral radius bounds [Nik06], combinatorics on words generated by automata [Lot83], or simple combinatorial problems like the number of length k sequences of moves of a king on an $n\times n$ chess board [Cve70]. A huge amount of publications exists in the field of theoretical chemistry, see, e.g., [Raz86]. In general, entry sums of matrix powers often appear in the analysis of iteration processes, e.g., in population genetics [Edw00]. Among other things, we will show further relations between walks and iterated kernels as well as directed line graphs.

First, we briefly review related work. Lagarias, Mazo, Shepp, and McKay [LMSM84] proved that the inequality $w_r \cdot w_s \le n\cdot w_{r+s}$ holds for the case of an even sum $r+s$. Hence, it could be stated as $w_{2a+b}\cdot w_b \le w_0 \cdot w_{2(a+b)}$ for $a,b\in\mathbb{N}$. (Furthermore, they presented counterexamples whenever $r+s$ is odd and $r,s\ge 1$.) A unification with the similar result $w^2_{a+b} \le w_{2a}\cdot w_{2b}$ by Dress and Gutman [DG03] was provided in [TWK+13]. Later, it was realized that this generalized form is a special case of the following theorem in which Marcus and Newman [MN62] considered inequalities of unweighted entry sums.

Theorem 1 (Marcus and Newman). *For every Hermitian matrix A and nonnegative integers $a,b,c\in\mathbb{N}$, the following inequality holds:*

$$\text{sum}\left(A^{2a+c}\right)\cdot\text{sum}\left(A^{2a+2b+c}\right) \le \text{sum}\left(A^{2a}\right)\cdot\text{sum}\left(A^{2(a+b+c)}\right) \quad .$$

Actually, Lagarias et al. did not only prove the inequality for the number of walks. They proved the more general real-weighted inequality $\left(v^TA^rv\right)\left(v^TA^sv\right) \le \left(v^Tv\right)\left(v^TA^{r+s}v\right)$ for *even* sum $r+s$, real symmetric matrix A, and real vector v. Thus, it could be stated as follows.

Theorem 2 (Lagarias, Mazo, Shepp, and McKay). *For any real symmetric $n\times n$-matrix A, real vector $\vec{s}\in\mathbb{R}^n$, and $a,b\in\mathbb{N}$ we have*

$$\left(\vec{s}^TA^{2a+b}\vec{s}\right)\left(\vec{s}^TA^{b}\vec{s}\right) \le \left(\vec{s}^T\vec{s}\right)\left(\vec{s}^TA^{2(a+b)}\vec{s}\right) \quad .$$

Those two theorems were unified and generalized by Täubig and Weihmann [TW12; TW14] to the following inequality with Hermitian matrix A, real weight vector $\vec{s}\in\mathbb{R}^n$, and $a,b,c\in\mathbb{N}$:

$$\left(\vec{s}^TA^{2a+c}\vec{s}\right)\left(\vec{s}^TA^{2a+2b+c}\vec{s}\right) \le \left(\vec{s}^TA^{2a}\vec{s}\right)\left(\vec{s}^TA^{2(a+b+c)}\vec{s}\right) \quad .$$

In this paper, we will generalize it to complex weight vectors in an appropriate way.

The related theorem $(\vec{s}^T A^k \vec{s})(\vec{s}^T \vec{s})^{k-1} \geq (\vec{s}^T A \vec{s})^k$ for nonnegative symmetric matrix A, nonnegative weight vector $\vec{s}$ and positive integer k was discovered by Mulholland and Smith [MS59], and later independently in slightly different form by Blakley and Roy [BR65]. This was used by Erdős and Simonovits [ES82] to deduce $w_k \geq n \cdot \overline{d}^k$, where $\overline{d}$ is the average degree of the graph. Using $w_1 = 2m$ and $w_0 = n$, this can also be written as $w_k \geq w_0(\frac{w_1}{w_0})^k$ or $w_1^k \leq w_0^{k-1} \cdot w_k$. The generalized form $w_{2\ell+p}^k \leq w_{2\ell}^{k-1} \cdot w_{2\ell+pk}$ for walk numbers was proposed in [TWK+13].

2 Hermitian Matrices and Undirected Graphs

2.1 The Complex-Weighted Sandwich Theorem

If A is a Hermitian matrix then the sum of all entries $(\mathbf{1}_n^T A \mathbf{1}_n)$ is a real number. Also the sum of all entries for any principal submatrix is a real number. In particular, this applies to each entry on the main diagonal.

More generally, we could try to sum up the entries of A or A^k in a weighted form where the entries of each row and every column are scaled by certain values. For instance, this method would allow to calculate the entry sum of a certain submatrix of A^k. In the context of walks of length k, we could filter the sets of start and end vertices by using the corresponding characteristic vectors of the vertex sets. By multiplying each row i and column i with the *same* scaling factor s_i, we obtain a Hermitian matrix again. Thus, using the quadratic form $\mathrm{sum}_{\vec{s}}(A) = \vec{s}^T A \vec{s} \in \mathbb{R}$ for $\vec{s} \in \mathbb{R}^n$, the weighted sum of all entries is again a real number. Of course, the same applies to the powers of the matrix, i.e., $\mathrm{sum}_{\vec{s}}\left(A^k\right) = \vec{s}^T A^k \vec{s} \in \mathbb{R}$ for $\vec{s} \in \mathbb{R}^n$. Using the *same* scaling vector for rows and columns allows us, for instance, to calculate the entry sum of a *principal* submatrix of A^k by using the characteristic vector of an index subset in place of $\vec{s}$.

This weighting scheme can be generalized even further to vectors of complex numbers by using Hermitian forms (or symmetric sesquilinear forms). A sesquilinear form on a complex vector space maps two argument vectors to a complex number in such a way that the mapping is linear in one argument and conjugate-linear (antilinear) in the other. A Hermitian form $h(x, y)$ is a sesquilinear form that satisfies $h(x, y) = \overline{h(y, x)}$. The standard Hermitian form is just the inner product $\langle x, y\rangle = \sum_{i=1}^n \bar{x}_i y_i$.[1] Note that the quadratic form $h(x, x)$ for any Hermitian form $h(x, y) = \overline{h(y, x)}$ is always real. In the following, we will consider the quadratic form $\mathrm{sum}_{\vec{s}}(A) = \vec{s}^* A \vec{s} = \langle \vec{s}, A\vec{s}\rangle \in \mathbb{R}$ for $\vec{s} \in \mathbb{C}^n$ and Hermitian matrix A.

By the spectral decomposition theorem, we know that each Hermitian matrix A can be diagonalized by a unitary matrix U, i.e., we have $A = UDU^*$, where D is a diagonal matrix containing the eigenvalues λ_i of A. Since A is Hermitian, all eigenvalues are real numbers. For matrix powers, we have $A^k = (UDU^*)^k = UD^kU^*$. The weighted sum of entries yields $\mathrm{sum}_{\vec{s}}\left(A^k\right) = \vec{s}^* A^k \vec{s} = \vec{s}^*(UDU^*)^k \vec{s} = \vec{s}^* U D^k U^* \vec{s} = \vec{c}_{\vec{s}}^{\,*} D^k \vec{c}_{\vec{s}}$, i.e., $\mathrm{sum}_{\vec{s}}\left(A^k\right) = \langle \vec{s}, A^k \vec{s}\rangle = \langle U^*\vec{s}, D^k U^* \vec{s}\rangle = \langle \vec{c}_{\vec{s}}, D^k \vec{c}_{\vec{s}}\rangle$ with $\vec{c}_{\vec{s}} = (c_{\vec{s},1}, \ldots, c_{\vec{s},n})^T = U^*\vec{s}$. We have $a_{x,y}^{[k]} = \left(A^k\right)_{(x,y)} = \sum_{i=1}^n u_{xi}\bar{u}_{yi}\lambda_i^k$. Since each entry in row x and column y will be weighted with the corresponding weights $\bar{s}_x$ and s_y, we define the following weighted version:

$$a_{x,y}^{[k,\vec{s}]} = \bar{s}_x s_y \left(A^k\right)_{(x,y)} = \bar{s}_x s_y \sum_{i=1}^n u_{xi}\bar{u}_{yi}\lambda_i^k \quad .$$

Now, we use the following generalized definitions for entry sums of matrix powers: For index $x \in [n]$, let $r_x^{[k],\vec{s}}$ denote the weighted sum of the terms $a_{x,y}^{[k]}$ over all $y \in [n]$:

$$r_x^{[k],\vec{s}} = \sum_{y=1}^n a_{x,y}^{[k,\vec{s}]} = \bar{s}_x \sum_{y=1}^n s_y \sum_{i=1}^n u_{xi}\bar{u}_{yi}\lambda_i^k = \bar{s}_x \sum_{i=1}^n u_{xi} c_{\vec{s},i} \lambda_i^k.$$

[1] Here, we used the physics convention with conjugate linearity in the first (x) and linearity in the second (y) argument.

Then, the total weighted sum of the entries is

$$\mathrm{sum}_{\vec{s}}\left(A^k\right) = \sum_{x=1}^{n} \bar{s}_x r_x^{[k],\vec{s}} = \sum_{x=1}^{n} \bar{s}_x \sum_{i=1}^{n} u_{xi} c_{\vec{s},i} \lambda_i^k = \sum_{i=1}^{n} c_{\vec{s},i} \bar{c}_{\vec{s},i} \lambda_i^k \ .$$

Note that $c_{\vec{s},i}\bar{c}_{\vec{s},i}$ is a nonnegative real number since it is the product of a complex number $c = a + ib \in \mathbb{C}$ $(a, b \in \mathbb{R})$ and its complex conjugate $\bar{c} = a - ib$, i.e., we have $c\bar{c} = (a + ib)(a - ib) = a^2 - i^2b^2 = a^2 + b^2$. Although $\mathrm{sum}_{\vec{s}}(A)$ is a function of a complex vector $\vec{s}$ and a complex matrix A, this (Hermitian) form yields only real function values for any Hermitian matrix A. The same applies to $\mathrm{sum}_{\vec{s}}\left(A^k\right)$.

Theorem 3. *For all Hermitian matrices A, nonnegative integers $a, b, c \in \mathbb{N}$, and complex weight vectors $\vec{s} \in \mathbb{C}^n$, the following inequality holds:*

$$\mathrm{sum}_{\vec{s}}\left(A^{2a+c}\right) \cdot \mathrm{sum}_{\vec{s}}\left(A^{2a+2b+c}\right) \leq \mathrm{sum}_{\vec{s}}\left(A^{2a}\right) \cdot \mathrm{sum}_{\vec{s}}\left(A^{2(a+b+c)}\right) \ .$$

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

$$\begin{aligned}
&\mathrm{sum}_{\vec{s}}\left(A^{2a}\right) \cdot \mathrm{sum}_{\vec{s}}\left(A^{2(a+b+c)}\right) - \mathrm{sum}_{\vec{s}}\left(A^{2a+c}\right) \cdot \mathrm{sum}_{\vec{s}}\left(A^{2a+2b+c}\right) \\
=\ & \sum_{i=1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}\lambda_i^{2a} \sum_{j=1}^{n} c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_j^{2(a+b+c)} - \sum_{i=1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}\lambda_i^{2a+c} \sum_{j=1}^{n} c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_j^{2a+2b+c} \\
=\ & \sum_{i=1}^{n}\sum_{j=1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}c_{\vec{s},j}\bar{c}_{\vec{s},j} \left(\lambda_i^{2a}\lambda_j^{2(a+b+c)} - \lambda_i^{2a+c}\lambda_j^{2a+2b+c}\right) \\
=\ & \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_i^{2a}\lambda_j^{2a} \left(\lambda_j^{2(b+c)} - \lambda_i^c\lambda_j^{2b+c} + \lambda_i^{2(b+c)} - \lambda_j^c\lambda_i^{2b+c}\right) \\
=\ & \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_i^{2a}\lambda_j^{2a} \left(\lambda_j^{2b+c} - \lambda_i^{2b+c}\right)\left(\lambda_j^c - \lambda_i^c\right).
\end{aligned}$$

Each term within the last line must be nonnegative, since $(c_{\vec{s},i}\bar{c}_{\vec{s},i})$, $(c_{\vec{s},j}\bar{c}_{\vec{s},j})$, λ_i^{2a}, and λ_j^{2a} are all nonnegative, and $(\lambda_j^{2b+c} - \lambda_i^{2b+c})$ and $(\lambda_j^c - \lambda_i^c)$ must have the same sign. □

The last argument means that the sequences $\{\lambda_i^{2b+c}\}$ and $\{\lambda_i^c\}$ are similarly ordered (because $2b+c$ and c must be either both odd or both even numbers). If all eigenvalues λ_i are nonnegative, then the proof also works for mixed odd/even powers:

Theorem 4. *For all positive-semidefinite matrices A, integers $a, b, c \in \mathbb{N}$, and weight vectors $\vec{s} \in \mathbb{C}^n$, the following inequality holds:*

$$\mathrm{sum}_{\vec{s}}\left(A^{a+b}\right) \cdot \mathrm{sum}_{\vec{s}}\left(A^{a+b+c}\right) \leq \mathrm{sum}_{\vec{s}}\left(A^{a}\right) \cdot \mathrm{sum}_{\vec{s}}\left(A^{a+2b+c}\right) \ .$$

Proof. The proof is essentially the same as for Theorem 3, except that squares of eigenvalues are not required as all eigenvalues are nonnegative in the case of positive-semidefinite matrices.

As in the proof of Theorem 3, we consider the difference of both sides of the inequality:

$$
\begin{aligned}
&\operatorname{sum}_{\vec{s}}\left(A^{a}\right) \cdot \operatorname{sum}_{\vec{s}}\left(A^{a+2b+c}\right) - \operatorname{sum}_{\vec{s}}\left(A^{a+b}\right) \cdot \operatorname{sum}_{\vec{s}}\left(A^{a+b+c}\right) \\
= &\sum_{i=1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}\lambda_i^{a} \sum_{j=1}^{n} c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_j^{a+2b+c} - \sum_{i=1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}\lambda_i^{a+b} \sum_{j=1}^{n} c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_j^{a+b+c} \\
= &\sum_{i=1}^{n}\sum_{j=1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}c_{\vec{s},j}\bar{c}_{\vec{s},j}\left(\lambda_i^{a}\lambda_j^{a+2b+c} - \lambda_i^{a+b}\lambda_j^{a+b+c}\right) \\
= &\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}c_{\vec{s},j}\bar{c}_{\vec{s},j}\Big(\lambda_i^{a}\lambda_j^{a+2b+c} - \lambda_i^{a+b}\lambda_j^{a+b+c} + \lambda_j^{a}\lambda_i^{a+2b+c} - \lambda_j^{a+b}\lambda_i^{a+b+c}\Big) \\
= &\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_i^{a}\lambda_j^{a}\Big(\lambda_j^{2b+c} - \lambda_i^{b}\lambda_j^{b+c} + \lambda_i^{2b+c} - \lambda_j^{b}\lambda_i^{b+c}\Big) \\
= &\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} c_{\vec{s},i}\bar{c}_{\vec{s},i}c_{\vec{s},j}\bar{c}_{\vec{s},j}\lambda_i^{a}\lambda_j^{a}\left(\lambda_j^{b+c} - \lambda_i^{b+c}\right)\left(\lambda_j^{b} - \lambda_i^{b}\right).
\end{aligned}
$$

Again, $(c_{\vec{s},i}\bar{c}_{\vec{s},i})$ and $(c_{\vec{s},j}\bar{c}_{\vec{s},j})$ are nonnegative numbers. Furthermore, $\lambda_i^a\lambda_j^a$ is nonnegative, and $(\lambda_j^{b+c} - \lambda_i^{b+c})$ and $(\lambda_j^b - \lambda_i^b)$ must have the same sign since $\lambda_i, \lambda_j \geq 0$. Therefore, each term within the last line must be nonnegative. ☐

The missing cases for negative-semidefinite matrices can be deduced from the last line of the previous proof.

Theorem 5. *For all negative-semidefinite matrices A, integers $a, b, c \in \mathbb{N}$, and weight vectors $\vec{s} \in \mathbb{C}^n$, the following inequalities hold.*

If c is even, we have

$$\operatorname{sum}_{\vec{s}}\big(A^{a+b}\big) \cdot \operatorname{sum}_{\vec{s}}\big(A^{a+b+c}\big) \leq \operatorname{sum}_{\vec{s}}\big(A^{a}\big) \cdot \operatorname{sum}_{\vec{s}}\big(A^{a+2b+c}\big) \quad .$$

If c is odd, we have

$$\operatorname{sum}_{\vec{s}}\big(A^{a+b}\big) \cdot \operatorname{sum}_{\vec{s}}\big(A^{a+b+c}\big) \geq \operatorname{sum}_{\vec{s}}\big(A^{a}\big) \cdot \operatorname{sum}_{\vec{s}}\big(A^{a+2b+c}\big) \quad .$$

Proof. We refer to the same transformation as in the previous proof. Again, $(c_{\vec{s},i}\bar{c}_{\vec{s},i})$, $(c_{\vec{s},j}\bar{c}_{\vec{s},j})$, and $\lambda_i^a\lambda_j^a$ are nonnegative. Now, the sequences $\{\lambda_i^b\}$ and $\{\lambda_i^{b+c}\}$ are similarly ordered if c is even (since $\lambda_i \leq 0$). They are conversely ordered if c is odd. ☐

2.2 Inequalities for Iterated Kernels

An *integral transform* is a mathematical operator T that obeys the form

$$(Tf)(u) = \int_{x_1}^{x_2} K(x,u)\, f(x)\, dx \quad .$$

In this way, it transforms the function f into a new function Tf. Each instance of an integral transform is specified by a particular choice for K. This function of two variables is called the *kernel function* of the integral transform. There are several popular examples of integral transforms like the Fourier transform, the Laplace transform, or the Mellin transform.

An *iterated kernel* is a function $K_i(x,s)$ that is formed from the given kernel $K(x,s)$ of an integral operator $Af(x) = \int_a^b K(x,t)\, f(t)\, dt$ by the recurrence relations $K_1(x,s) = K(x,s)$ and $K_i(x,s) = \int_a^b K_{i-1}(x,t)K(t,s)\, dt$. The function K_i is called the i-th iterated kernel of K. The kernel K_i is the kernel of the operator A^i. The equality $K_i(x,s) = \int_a^b K_{i-j}(x,t)K_j(t,s)\, dt$ holds for $1 \leq j \leq i-1$.

From Theorem 3, we conclude the following by Riemann approximation of the integrals.

Corollary 6. *For any symmetric kernel K and any function v, we have*

$$\begin{aligned}&\int_0^a\int_0^a v(x)v(y)K_{2a+c}(x,y)\,dx\,dy\int_0^a\int_0^a v(x)v(y)K_{2a+2b+c}(x,y)\,dx\,dy\\ \leq\ &\int_0^a\int_0^a v(x)v(y)K_{2a}(x,y)\,dx\,dy\int_0^a\int_0^a v(x)v(y)K_{2(a+b+c)}(x,y)\,dx\,dy\ .\end{aligned}$$

For the unweighted case, we have

$$\begin{aligned}&\int_0^a\int_0^a K_{2a+c}(x,y)\,dx\,dy\int_0^a\int_0^a K_{2a+2b+c}(x,y)\,dx\,dy\\ \leq\ &\int_0^a\int_0^a K_{2a}(x,y)\,dx\,dy\int_0^a\int_0^a K_{2(a+b+c)}(x,y)\,dx\,dy\ .\end{aligned}$$

Inequalities of this kind are useful, e.g., in the context of mathematical population genetics, see [MPF91; Edw00].

2.3 Counterexamples for Further Conceivable Inequalities

By giving counterexamples, Lagarias et al. [LMSM84] disproved the inequality $w_r \cdot w_s \leq n \cdot w_{r+s}$ for all pairs (r, s) where the sum $r + s$ takes an odd value. Those counterexamples are disconnected graphs consisting of a complete graph K_{m+1} and a star S_{m^2+t+1} for $t \geq 1$ and m sufficiently large. Connected counterexamples can be constructed by adding an edge between a vertex of the complete subgraph and a leaf of the star.

We will reuse the method of Lagarias et al. and try to construct counterexamples for other possible inequalities. In particular, we are looking for counterexamples to the following conceivable sandwich inequality:

$$w_{a+c} \cdot w_{a+2b+c+1} \overset{?}{\leq} w_a \cdot w_{a+2b+2c+1}\ .$$

As can be seen, each side consists of a product involving one *even* and one *odd* walk length. Again, the graphs we consider consist of a complete graph K_{m+1} and a star S_{m^2+t+1} for $t \geq 1$. For the number of walks of the star part, we have to distinguish between even and odd walk lengths. For a star on n nodes, we have $w_{2i} = n(n-1)^i$ and $w_{2i+1} = 2(n-1)^{i+1}$. For a complete graph on n nodes, we have $w_i = n(n-1)^i$. Note that in any case we have $w_{a+c}(G_i)w_{a+2b+c+1}(G_i) = w_a(G_i)w_{a+2b+2c+1}(G_i)$ for each of the two subgraphs $G_1 = K_{m+1}$ and $G_2 = S_{m^2+t+1}$. Thus, only the mixed terms need to be considered for the difference.

From now, we assume that a is even and $a + 2b + 2c + 1$ is odd. (This specific approach does not yield counterexamples when a is odd.) Now, we distinguish the two cases for c. First, we assume that c is odd ($a + c$ odd, $a + 2b + c + 1$ even). Thus, we have

$$\begin{array}{ccrcc} & & K_{m+1} & & S_{m^2+t+1} \\ w_{a+c} & = & m^{a+c}(m+1) & + & 2(m^2+t)^{(a+c+1)/2} \\ w_{a+2b+c+1} & = & m^{a+2b+c+1}(m+1) & + & (m^2+t)^{(a+2b+c+1)/2}(m^2+t+1) \\ w_a & = & m^a(m+1) & + & (m^2+t)^{a/2}(m^2+t+1) \\ w_{a+2b+2c+1} & = & m^{a+2b+2c+1}(m+1) & + & 2(m^2+t)^{(a+2b+2c+2)/2}\ . \end{array}$$

For the difference $w_{a+c}w_{a+2b+c+1} - w_a w_{a+2b+2c+1}$, we obtain $m^{a+c}(m+1)\cdot(m^2+t)^{(a+2b+c+1)/2}(m^2+t+1)+m^{a+2b+c+1}(m+1)\cdot 2(m^2+t)^{(a+c+1)/2} - m^a(m+1)\cdot 2(m^2+t)^{(a+2b+2c+2)/2} - m^{a+2b+2c+1}(m+$

$1) \cdot (m^2+t)^{a/2}(m^2+t+1)$, i.e.,

$$\begin{aligned}
&(w_{a+c}w_{a+2b+c+1} - w_a w_{a+2b+2c+1})/(m^a(m+1)(m^2+t)^{a/2}) \\
&\quad = \; m^c(m^2+t+1)\left[(m^2+t)^{(2b+c+1)/2} - m^{2b+c+1}\right] \\
&\qquad +2(m^2+t)^{(c+1)/2}\left[m^{2b+c+1} - (m^2+t)^{(2b+c+1)/2}\right] \\
&\quad = \; \left[m^c(m^2+t+1) - 2(m^2+t)^{(c+1)/2}\right] \cdot \left[(m^2+t)^{(2b+c+1)/2} - m^{2b+c+1}\right] \\
&\quad = \; \left[m^{c+2} + m^c(t+1) - 2(m^2+t)^{(c+1)/2}\right] \cdot \left[(m^2+t)^{(2b+c+1)/2} - m^{2b+c+1}\right] \; .
\end{aligned}$$

By the binomial theorem, we have $(m^2+t)^{(2b+c+1)/2} - m^{2b+c+1} > 0$ and $2(m^2+t)^{(c+1)/2} \in \mathcal{O}(m^{c+1})$. Therefore, the difference must be strictly positive for fixed $t \geq 1$ and sufficiently large m.

For the second case, we assume that a is even ($a+2b+2c+1$ odd), c even ($a+c$ even , $a+2b+c+1$ odd):

$$\begin{array}{rcrcl}
 & & K_{m+1} & & S_{m^2+t+1} \\
w_{a+c} & = & m^{a+c}(m+1) & + & (m^2+t)^{(a+c)/2}(m^2+t+1) \\
w_{a+2b+c+1} & = & m^{a+2b+c+1}(m+1) & + & 2(m^2+t)^{(a+2b+c+2)/2} \\
w_a & = & m^a(m+1) & + & (m^2+t)^{a/2}(m^2+t+1) \\
w_{a+2b+2c+1} & = & m^{a+2b+2c+1}(m+1) & + & 2(m^2+t)^{(a+2b+2c+2)/2} \; .
\end{array}$$

For the difference $w_{a+c}w_{a+2b+c+1} - w_a w_{a+2b+2c+1}$, we obtain $m^{a+c}(m+1)\cdot 2(m^2+t)^{(a+2b+c+2)/2} + m^{a+2b+c+1}(m+1)\cdot(m^2+t)^{(a+c)/2}(m^2+t+1) - m^a(m+1)\cdot 2(m^2+t)^{(a+2b+2c+2)/2} - m^{a+2b+2c+1}(m+1)\cdot(m^2+t)^{a/2}(m^2+t+1)$, i.e.,

$$\begin{aligned}
&(w_{a+c}w_{a+2b+c+1} - w_a w_{a+2b+2c+1})/(m^a(m+1)(m^2+t)^{a/2}) \\
&\quad = \; m^{2b+c+1}(m^2+t+1)\left[(m^2+t)^{c/2} - m^c\right] \\
&\qquad +2(m^2+t)^{(2b+c+2)/2}\left[m^c - (m^2+t)^{c/2}\right] \\
&\quad = \; \left[m^{2b+c+1}(m^2+t+1) - 2(m^2+t)^{(2b+c+2)/2}\right] \cdot \left[(m^2+t)^{c/2} - m^c\right] \\
&\quad = \; \left[m^{2b+c+3} + m^{2b+c+1}(t+1) - 2(m^2+t)^{(2b+c+2)/2}\right] \cdot \left[(m^2+t)^{c/2} - m^c\right] \; .
\end{aligned}$$

By the binomial theorem, we have $(m^2+t)^{c/2} - m^c > 0$ and $2(m^2+t)^{(2b+c+2)/2} \in \mathcal{O}(m^{2b+c+2})$. Therefore, the difference must be strictly positive for fixed $t \geq 1$ and sufficiently large m.

In summary, we can state the following for the case of odd-times-even lengths on both sides when a is even ($a = 2a'$).

Theorem 7. *For $a', b, c \in \mathbb{N}$, there are graphs with*

$$w_{2a'+c} \cdot w_{2a'+2b+c+1} \not\leq w_{2a'} \cdot w_{2a'+2b+2c+1} \; .$$

3 Bounds for the Largest Eigenvalue

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

In several other papers, the sum of squares of walk numbers was considered to obtain the lower bounds $\sum_{v\in V} w_2(v)^2/\sum_{v\in V} d_v^2 \leq \lambda_1^2$ [YLT04], $\sum_{v\in V} w_3(v)^2/\sum_{v\in V} w_2(v)^2 \leq \lambda_1^2$ [HZ05], $\sum_{v\in V} w_4(v)^2/\sum_{v\in V} w_3(v)^2 \leq \lambda_1^2$ [Hu09], and $\sum_{v\in V} w_{k+1}(v)^2/\sum_{v\in V} w_k(v)^2 \leq \lambda_1^2$ [HTW07]. These inequalities correspond to the following statements:

$$\frac{w_4}{w_2} \leq \lambda_1^2 \; , \qquad \frac{w_6}{w_4} \leq \lambda_1^2 \; , \qquad \frac{w_8}{w_6} \leq \lambda_1^2 \; , \qquad \text{and} \qquad \frac{w_{2k+2}}{w_{2k}} \leq \lambda_1^2 \; .$$

These results were generalized by Nikiforov [Nik06] as follows.[2]

Theorem 8 (Nikiforov)**.** *For each undirected graph and $k, r \in \mathbb{N}$, we have*

$$\frac{w_{2k+r}}{w_{2k}} \leq \lambda_1^r \ ,$$

where λ_1 is the largest eigenvalue of the adjacency matrix of the graph.

Note that this theorem follows already from a result of Hyyrö, Merikoski, and Virtanen [HMV86]. Nikiforov additionally characterized the case of equality. Here, we propose the following generalization.

Theorem 9. *For any normal matrix B with spectral radius $\rho(B)$ and $x, y \in \mathbb{C}^n$, we have*

$$|x^* B y| \leq \rho(B) \sqrt{x^* x} \sqrt{y^* y} \ .$$

Proof. By the Cauchy-Schwarz inequality, we have

$$|x^* B y| = |\langle x, By \rangle| \leq \sqrt{|\langle x, x \rangle|} \sqrt{|\langle By, By \rangle|} = \sqrt{x^* x} \sqrt{y^* B^* B y} \ .$$

Note that $B^* B$ is a positive-semidefinite Hermitian matrix. By the Rayleigh-Ritz Theorem, we know that

$$\frac{y^* B^* B y}{y^* y} \leq \lambda_{\max}(B^* B) \ ,$$

where $\lambda_{\max}(B^* B)$ denotes the largest eigenvalue of the matrix $B^* B$.

Now we are looking for a connection between $\lambda_{\max}(B^* B)$ and the eigenvalues of B. Since B is a normal matrix, there is a spectral decomposition $B = U^* D U$ with diagonal matrix D containing the eigenvalues of B. Since $B^* = (U^* D U)^* = U^* D^* U$, we have $B^* B = U^* D U U^* D^* U = U^* (D D^*) U$, i.e., the eigenvalues of $B^* B$ are the values $\lambda_i \bar{\lambda_i}$ for $i = \{1, \ldots n\}$. Those values are just the squares of the absolute value (modulus) of each eigenvalue. Thus we have

$$\frac{y^* B^* B y}{y^* y} \leq \lambda_1(B^* B) = [\rho(B)]^2$$

and therefore $|x^* B y| \leq \rho(B) \sqrt{x^* x} \sqrt{y^* y}$. □

If B is a Hermitian matrix, then all the eigenvalues λ_i are real and the eigenvalues of $B^* B$ are just the squared eigenvalues of B. Then the largest eigenvalue of $B^* B$ is just $\max\{\lambda_1^2, \lambda_n^2\}$. If B is a nonnegative symmetric matrix, then we know (by the Perron-Frobenius Theorem) that the largest eigenvalue equals the spectral radius. If we consider an undirected graph with (symmetric) adjacency matrix A, we can set $B = A^r$, $x = A^a \mathbf{1}$, and $y = A^b \mathbf{1}$. Then we obtain the following corollary.

Corollary 10. *For all undirected graphs and $a, b, r \in \mathbb{N}$, we have*

$$\frac{w_{a+r+b}}{\sqrt{w_{2a} w_{2b}}} \leq \lambda_1^r \ .$$

Proof. The result follows from setting $B = A^r$ and from the fact that (by the Perron-Frobenius Theorem) the largest eigenvalue equals the spectral radius. Setting $a = b = k$ leads to $\frac{w_{2k+r}}{w_{2k}} \leq \lambda_1^r$, i.e., Nikiforov's inequality. □

[2]Note that Nikiforov defined w_k and the length of a walk in terms of the number of nodes instead of the number of edges.

4 Iterated Directed Line Graphs

The (undirected) line graph $\mathcal{L}(G)$ of a graph $G = (V, E)$ is a graph where each edge $e \in E$ of G is represented by a vertex v_e in $\mathcal{L}(G)$, i.e., there is a one-to-one mapping between the edges of G and the vertices of $\mathcal{L}(G)$. For edges $e, f \in E$, there is an edge between the corresponding vertices v_e and v_f in the line graph $\mathcal{L}(G)$ if and only if e and f share *exactly one* vertex in G.

The directed line graph or line digraph $\mathcal{LD}(G)$ of a directed graph $G = (V, E)$ is the directed graph that has a vertex v_e for each edge e of G. Two vertices v_1 and v_2 of the line digraph representing the original edges (s_1, t_1) and (s_2, t_2) are connected by an edge (v_1, v_2) in the line digraph if and only if $t_1 = s_2$.The line digraph of an undirected graph is defined as the line digraph of its corresponding bidirected graph (using antiparallel edges for each undirected edge). Note that the line digraph of an undirected graph G is related to but *not the same* as the graph that results from the undirected line graph of G by replacing the undirected edges by antiparallel directed edges. The reason is that the (self-)loops of the line digraphs (representing walks of length 2 traversing the same edge forward and backward) are not present in the undirected line graph.

If we repeat the operation of constructing the line digraph of a graph, this process yields the k-th iterated line digraph. For convenience, we define $\mathcal{LD}_0(G) = G$. Starting with $\mathcal{LD}_1(G) = \mathcal{LD}(G)$, the process continues recursively using $\mathcal{LD}_{k+1}(G) = \mathcal{LD}(\mathcal{LD}_k(G))$.

Note that the edges of the line digraph $\mathcal{LD}(G)$ represent exactly the walks of length 2 in the original digraph G (while the vertices correspond to the edges, i.e., to the walks of length 1). Here the question arises whether there is a more general relation between the nodes or edges in an iterated line digraph and the walks in the original digraph. At first, one might suspect that repeating the operation leads to doubling the walk length with every iteration, but this is not true. As shown in following theorem, the walk length is incremented by one in each iteration. Note that this observation is also implicitly contained in the paper by Levine [Lev11].

Theorem 11. *The vertices of the k-th iterated directed line graph of a graph G are in one-to-one correspondence with the walks of length k in G. The edges of $\mathcal{LD}_k(G)$ correspond to the walks of length $k+1$ in G.*

Proof. For $\mathcal{LD}_0(G) = G$, the statement is obvious. As already mentioned, we know for $\mathcal{LD}_1(G) = \mathcal{LD}(G)$ that the vertices correspond to the edges of G, i.e., to the walks of length 1. The edges in $\mathcal{LD}(G)$ connect exactly the vertices of $\mathcal{LD}(G)$ that are represented by original edges (s_1, t_1) and (s_2, t_2) with $t_1 = s_2$. Therefore, they represent exactly the walks of length 2: $(s_1, t_1, t_2) = (s_1, s_2, t_2)$. Now, the proof can be done by induction using the same principle for longer walks. Assume that the statement is true for $k = \ell$. Since the vertices of $\mathcal{LD}_{\ell+1}(G) = \mathcal{LD}(\mathcal{LD}_\ell(G))$ correspond to the edges of $\mathcal{LD}_\ell(G)$ and there is a bijection between the edges of $\mathcal{LD}_\ell(G)$ and the walks of length $\ell + 1$ in G, there must be a bijection between the vertices of $\mathcal{LD}_{\ell+1}(G)$ and the $(\ell + 1)$-walks in G. Consider two vertices x and y in $\mathcal{LD}_{\ell+1}(G)$. They represent $(\ell + 1)$-walks w_x and w_y and they correspond to edges (s_x, t_x) and (s_y, t_y) in $\mathcal{LD}_\ell(G)$. Here s_x, t_x, s_y, and t_y correspond to ℓ-walks in G. The vertices x and y are connected by a directed edge (x, y) in $\mathcal{LD}_{\ell+1}(G)$ if and only if $t_x = s_y$, i.e., the $(\ell + 1)$-walks w_x and w_y overlap in the ℓ-walk $t_x = s_y$. Hence, each such edge (x, y) corresponds to a walk of length $k+2$. Thus, the statement also holds for $k = \ell + 1$, and therefore for all $k \in \mathbb{N}$. $\square$

Corollary 12. *The number of nodes in $\mathcal{LD}^k(G)$ equals w_k, i.e., the number of walks of length k in G. The number of edges in $\mathcal{LD}^k(G)$ equals w_{k+1}.*

We can also state this in another form: For the number of walks of length k in the ℓ-th iterated directed line graph, we have $w_k(\mathcal{LD}^\ell(G)) = w_{k+\ell}(G)$.

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