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Chebyshev's Sum Inequality and the Zagreb Indices Inequality

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Abstract

In a recent article, Nadeem and Siddique used Chebyshev's sum inequality to establish the Zagreb indices inequality $M_1/n \leq M_2/m$ for undirected graphs in the case where the degree sequence (d_i) and the degree-sum sequence (S_i) are similarly ordered. We show that this is actually not a completely new result and we discuss several related results that also cover similar inequalities for directed graphs, as well as sum-symmetric matrices and Eulerian directed graphs.

1 Introduction

1.1 Notation

We consider $n \times n$ matrices, denoted by A, with entries a_{ij}. In particular, we look at the total sum of entries denoted by $\mathrm{sum}(A)$, as well as the row and column sums of A, which are denoted by $r_i(A)$ and $c_j(A)$, respectively. If A is clear from the context, we abbreviate this by r_i and c_j. For the matrix power A^p, $p \in \mathbb{N}$, we define the following abbreviations: $a_{ij}^{[p]} := (A^p)_{ij}$, $r_i^{[p]} := r_i(A^p)$, and $c_j^{[p]} := c_j(A^p)$. We assume that $A^0 = I$ is the identity matrix.

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As a special case, we consider adjacency matrices of directed and undirected (multi-)graphs $G = (V, E)$ with $n := |V|$ vertices and $m := |E|$ edges. The in-degree and the out-degree of a vertex $v \in V$ are denoted by $d_{\mathrm{in}}(v)$ and $d_{\mathrm{out}}(v)$, respectively. In undirected graphs, the degree of a vertex $v \in V$ is denoted by $d(v)$. A *walk* in a multigraph $G = (V, E)$ is an alternating sequence $(v_0, e_1, v_1, \ldots, v_{k-1}, e_k, v_k)$ of vertices $v_i \in V$ and edges $e_i \in E$ where each edge e_i of the walk must connect vertex v_{i-1} to vertex v_i in G, that is, $e_i = (v_{i-1}, v_i)$ for all $i \in \{1, \ldots, k\}$. Vertices and edges can be used repeatedly in the same walk. If the multigraph has no parallel edges, then the walks could also be specified by the sequence of vertices $(v_0, v_1, \ldots, v_{k-1}, v_k)$ without the edges. The *length* of a walk is the number of edge traversals. That means, the walk $(v_0, \ldots, v_k)$ consisting of $k + 1$ vertices and k edges is a walk of length k. We call it a *k-step walk*. Let $s_k(v)$ denote the number of k-step walks starting at vertex $v \in V$ and let $e_k(v)$ denote the number of k-step walks ending at v. If G is undirected, then we have $w_k(v) := s_k(v) = e_k(v)$. The total number of k-step walks is denoted by w_k. For walks of length 0, we have $s_0(v) = e_0(v) = 1$ for each vertex v and $w_0 = n$. For walks of length 1, we have $s_1(v) = d_{\mathrm{out}}(v)$ and $e_1(v) = d_{\mathrm{in}}(v)$, i.e., $w_1(v) = d(v)$ for undirected graphs. This implies $w_1 = \sum_{v \in V} d_{\mathrm{out}}(v) = \sum_{v \in V} d_{\mathrm{in}}(v) = m$ for directed graphs. For undirected graphs, we have $w_1 = \sum_{v \in V} d(v) = 2m$ by the handshake lemma.

1.2 Chebyshev's sum inequality

Two n-tuples $(a_1, \ldots, a_n)$ and $(b_1, \ldots, b_n)$ of real numbers are called *similarly ordered* if $(a_i - a_k)(b_i - b_k) \geq 0$ for all $i, k \in [n]$. They are called *conversely ordered* (also *oppositely ordered*, see [9]) if $(a_i - a_k)(b_i - b_k) \leq 0$ for all $i, k = 1, \ldots, n$. The term similarly ordered is equivalent to the requirement that there exists a permutation that transforms both tuples into nonincreasing sequences. In the same line, two tuples are conversely ordered if and only if there is a permutation that transforms one of the tuples into a nonincreasing and the other tuple into a nondecreasing sequence. Below, we will use the same notation for n-dimensional real vectors $a, b \in \mathbb{R}^n$.

The following inequality was published by Chebyshev [3, 13].

Theorem 1 (Chebyshev)**.** *Let* $f, g : [a, b] \mapsto \mathbb{R}$ *be integrable functions, both non-decreasing or both non-increasing. Furthermore, let* $p : [a, b] \mapsto \mathbb{R}_{\geq 0}$ *be an integrable nonnegative function. Then*

$$\int_a^b p(x)\, dx \int_a^b p(x) f(x) g(x)\, dx \geq \int_a^b p(x) f(x)\, dx \int_a^b p(x) g(x)\, dx \ .$$

If one of the functions f *or* g *is non-decreasing and the other non-increasing, then the sign of inequality is reversed.*

The discrete analog is the following statement.

Corollary. *For similarly ordered vectors* $a \in \mathbb{R}^n$ *and* $b \in \mathbb{R}^n$ *and any nonnegative vector* $p \in \mathbb{R}^n_{\geq 0}$*, we have*

$$\left(\sum_{i=1}^{n} p_i a_i\right)\left(\sum_{i=1}^{n} p_i b_i\right) \leq \left(\sum_{i=1}^{n} p_i\right)\left(\sum_{i=1}^{n} p_i a_i b_i\right) \ .$$

The inequality is reversed if a *and* b *are conversely ordered.*

If $p \in \mathbb{R}^n_{\geq 0}$ is nonzero, this corresponds to the following weighted arithmetic means relation:

$$\frac{\sum_{i=1}^n p_i a_i}{\sum_{i=1}^n p_i} \cdot \frac{\sum_{i=1}^n p_i b_i}{\sum_{i=1}^n p_i} \leq \frac{\sum_{i=1}^n p_i a_i b_i}{\sum_{i=1}^n p_i} \ .$$

A direct consequence is the following. Given $a, b \in \mathbb{R}^n$ and $r \in \mathbb{R}$, suppose that a_i^r and b_i^r are defined within $\mathbb{R}$ for all $i \in [n]$ and that the corresponding tuples $(a_1^r, \ldots, a_n^r)$ and $(b_1^r, \ldots, b_n^r)$ are similarly ordered. Then we have

$$\frac{\sum_{i=1}^n p_i a_i^r}{\sum_{i=1}^n p_i} \cdot \frac{\sum_{i=1}^n p_i b_i^r}{\sum_{i=1}^n p_i} \leq \frac{\sum_{i=1}^n p_i (a_i b_i)^r}{\sum_{i=1}^n p_i} \ .$$

One particular case where such inequalities can be obtained occurs for *arbitrary* exponents r and *nonnegative* vectors a and b that are similarly or conversely ordered. Another special case is for *odd integer* exponents r (or their reciprocals) and *arbitrary* real vectors a and b.

Corollary. *If the vectors* $a \in \mathbb{R}^n$ *and* $b \in \mathbb{R}^n$ *are similarly ordered, then*

$$\left(\sum_{i=1}^{n} a_i\right)\left(\sum_{i=1}^{n} b_i\right) \leq n \sum_{i=1}^{n} a_i b_i \ .$$

The inequality is reversed if a *and* b *are conversely ordered.*

For $n > 0$, this is the same as the following relation between arithmetic means:

$$\frac{\sum_{i=1}^{n} a_i}{n} \cdot \frac{\sum_{i=1}^{n} b_i}{n} \leq \frac{\sum_{i=1}^{n} a_i b_i}{n} \ .$$

All those variants are called Chebyshev's (sum) inequality.

2 Zagreb indices and walks

2.1 The Zagreb indices inequality

The first and the second *Zagreb [group] index* for an undirected graph $G = (V, E)$ are defined as[†]

$$M_1 = \sum_{v \in V} d_v^2 \qquad \text{and} \qquad M_2 = \sum_{\{x,y\} \in E} d_x d_y \ .$$

Assume that $V = \{v_1, \ldots, v_n\}$ and that the vertex degrees are abbreviated by $d_i = d(v_i)$. Recently, an article was published by Nadeem and Siddique [14] that contains the following statement concerning the degree-sums $S_i := \sum_{v_j \in N(v_i)} d(v_j)$, where $N(v_i) := \{v_j \in V \mid \{v_i, v_j\} \in E\}$ is the set of neighbors of v_i.

Theorem 2. *Let* G *be a connected graph having degree sequence* (d_i)*, degree-sum sequence* (S_i)*, order* n *and size* m*. If* (d_i) *and* (S_i) *are similarly ordered, then*

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \ .$$

[†]The first explicit definition of those indices appeared in the paper by Gutman et al. [6]. Erroneously, it referred to the earlier article by Gutman and Trinajstić [7] as the point where these measures where introduced. Actually, this is not true. This historical development was clarified recently by Gutman [4].

Equality is attained if and only if G is a regular or a complete bipartite graph.

They also remark for the part with the sufficient condition, that the Zagreb indices inequality holds for both, connected and non-connected graphs.

That means, this result uses Chebyshev's sum inequality to establish the Zagreb indices inequality in the case where the sequences (d_i) and (S_i) are similarly ordered.

2.2 The number of walks form

For a long time during the research on topological indices in chemical graph theory, it has been overlooked that two of the most popular descriptors were in fact just special cases of measures defined by the number of walks. Only after decades, it was observed by Nikolić et al. [15] and Braun et al. [2] that $M_1 = w_2$ (which is also implicitly contained in the paper by Gutman et al. [5], but not explicitly stated there) and that $M_2 = w_3/2$.

Together with $n = w_0$ and $m = w_1/2$, the Zagreb indices inequality can be rephrased as

$$w_2/w_0 \leq w_3/w_1 \ .$$

In the same line, we observe that the degree-sum S_i equals the number of 2-step walks starting at v_i, i.e., $S_i = w_2(v_i)$. And as already noted, we have $d_i = w_1(v_i)$.

In this respect, Theorem 2 can also be expressed as a statement about walks:

Theorem 3. *Let G be a graph having number of 1-step walks sequence $(w_1(v_i))$ and number of 2-step walks sequence $(w_2(v_i))$. If $(w_1(v_i))$ and $(w_2(v_i))$ are similarly ordered, then*

$$w_2/w_0 \leq w_3/w_1 \ .$$

Actually, this is not a new result. It is a special case of a more general theorem by Täubig [16, 18], see the corollary of Theorem 4 in the next section. Note also that a related observation corresponding to the Zagreb indices inequality has already been made by London [12] in the more general case of entry sums of nonnegative symmetric matrices.

The Zagreb indices inequality has been shown to hold for several special graph classes, such as trees [1, 21], chemical graphs [8], or subdivision graphs [10,17], while it does not hold for connected graphs in general [8,11] or for bipartite graphs, not even for forests (see Chapter 5 of [16] or [18]).

3 Applying Chebyshev's sum inequality to directed graphs

In order to obtain inequalities for the number of walks in directed graphs and for entry sums in nonsymmetric matrices, it is sometimes possible to apply Chebyshev's sum inequality. In those cases we are able to obtain statements by elementary proofs without using any eigenvalues.

Theorem 4. *For any matrix A such that the column sums of A^k and the row sums of A^ℓ (i.e., $c^{[k]}$ and $r^{[\ell]}$) are similarly ordered, we have*

$$\operatorname{sum}\left(A^k\right) \cdot \operatorname{sum}\left(A^\ell\right) \leq n \cdot \operatorname{sum}\left(A^{k+\ell}\right) \quad .$$

The inequality is reversed if $c^{[k]}$ and $r^{[\ell]}$ are conversely ordered.

Proof. For every $n \times n$ matrix A, we have

$$\operatorname{sum}\left(A^{k+\ell}\right) = \mathbf{1}_n^T \left(A^k A^\ell\right) \mathbf{1}_n = \left(\mathbf{1}_n^T A^k\right)\left(A^\ell \mathbf{1}_n\right) = \sum_{i \in [n]} c_i^{[k]} \cdot r_i^{[\ell]} \quad .$$

The inequality is now a direct consequence of Theorem 1:

$$\begin{aligned} \operatorname{sum}\left(A^k\right) \cdot \operatorname{sum}\left(A^\ell\right) &= \left(\sum_{i=1}^n c_i^{[k]}\right)\left(\sum_{i=1}^n r_i^{[\ell]}\right) \\ &\leq n \sum_{i=1}^n c_i^{[k]} r_i^{[\ell]} = n \cdot \operatorname{sum}\left(A^{k+\ell}\right) \quad . \end{aligned}$$

■

Note that for all Hermitian matrices A and integers k, ℓ where $k+\ell$ is an even number, Theorem 4 holds in general without the ordering assumption. Those inequalities and related results for real symmetric matrices and walks in undirected graphs were discussed in [20] and [19].

For the special case of adjacency matrices, Theorem 4 translates to the following statement about the number of walks in digraphs.

Corollary. *For every directed graph $G = (V, E)$ where the vectors of walk numbers $e_k(v)$ and $s_\ell(v)$, $v \in V$, are similarly ordered, we have*

$$w_k \cdot w_\ell \leq n \cdot w_{k+\ell} \ .$$

Obviously, this inequality is applicable to undirected graphs if $w_k(v_i)$ and $w_\ell(v_i)$, $i \in [n]$, are similarly ordered sequences (here, we have $w_k(v_i) = s_k(v_i) = e_k(v_i)$ for all $i, k \in \mathbb{N}$). In particular, this is interesting if $k + \ell$ is an odd number.

Inverted inequality: According to Chebyshev's sum inequality (see Theorem 1), the inequality is inverted if $e_k(v_i)$ and $s_\ell(v_i)$ are conversely ordered. For instance, this would be applicable for $k = \ell = 1$ if for each vertex either the in-degree or the out-degree is equal to 1 and the other one is greater or equal to 1. Another example would be the class of graphs where all vertices have the same sum of the in-degree and the out-degree (that is, the same total degree).

Sum-symmetric matrices: From Theorem 4, we obtain a special case if the row sums and the column sums of a matrix are similarly ordered. This happens, for example, in the case of sum-symmetric matrices, i.e., if $r_i(A) = c_i(A)$ for all $i \in [n]$.

Corollary. *For any sum-symmetric matrix A, we have*

$$\mathrm{sum}(A)^2 \leq n \cdot \mathrm{sum}(A^2) \ .$$

Note that this corollary also follows from Cauchy's inequality:

$$\mathrm{sum}(A)^2 = \left(\sum_{i=1}^{n} r_i\right)^2 \le n\sum_{i=1}^{n} r_i^2 = n\sum_{i=1}^{n} r_i c_i = n \cdot \mathrm{sum}(A^2) .$$

Eulerian directed graphs: We can apply this result to directed graphs as follows. If there is a vertex ordering which is monotonically increasing with respect to the in- and out-degrees, then the graph obeys the inequality $nw_2 \ge w_1^2$. For instance, this is true if the in-degree of each vertex equals its out-degree.

Corollary. *For every Eulerian directed graph ($\forall v \in V : d_{in}(v) = d_{out}(v)$), we have*

$$w_1^2 \le n \cdot w_2 \qquad \textit{or} \qquad w_1/w_0 \le w_2/w_1 .$$

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